Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:13 AM EDT

PDB ID	:	6DHC
Title	:	X-ray structure of BACE1 in complex with a bicyclic isoxazoline carboxamide as the P3 ligand
Authors	:	Mesecar, A.D.; Lendy, E.K.
Deposited on	:	2018-05-19
Resolution	:	2.85 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:

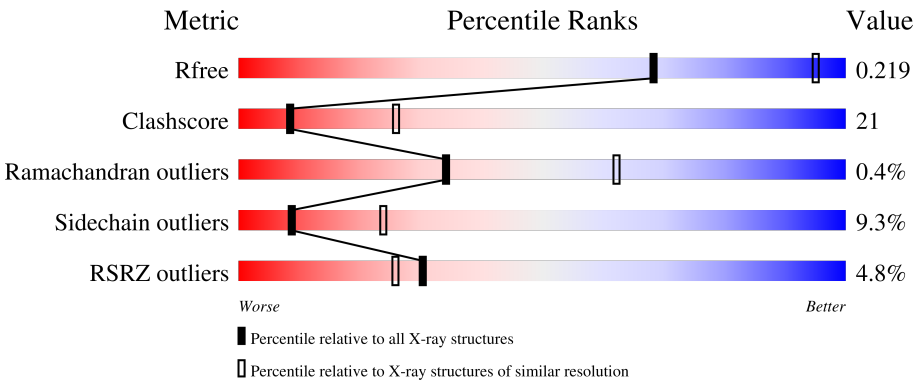
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	441	2%, 49%, 35%, •, 14%
1	B	441	7%, 49%, 33%, 5%, 14%
1	C	441	3%, 54%, 28%, •, 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GHJ	A	401	X	-	-	-
3	GOL	C	402	-	-	X	-
3	GOL	C	404	-	-	X	X

2 Entry composition (i)

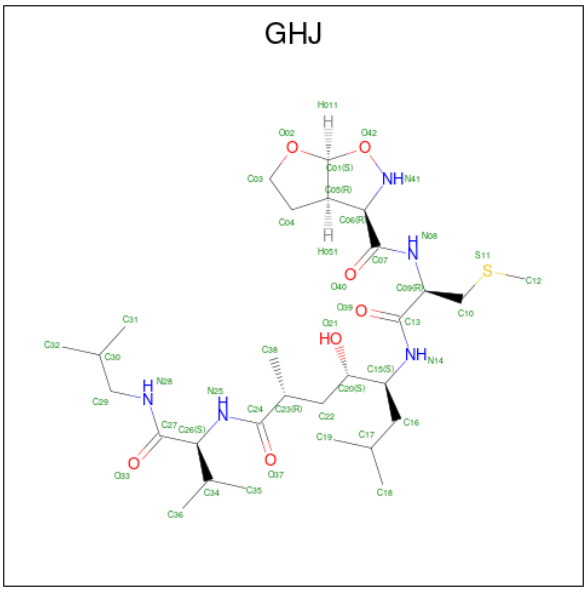
There are 6 unique types of molecules in this entry. The entry contains 9517 atoms, of which 153 are hydrogens and 0 are deuteriums.

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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	2970	1900	494	562	14	0	0	0
1	B	380	2983	1909	496	564	14	0	0	0
1	C	377	2965	1897	493	561	14	0	0	0

- Molecule 2 is (3R,3aR,6aS)-N-[(4R,7S,8S,10R,13S)-8-hydroxy-10,17-dimethyl-7-(2-methylpropyl)-5,11,14-trioxo-13-(propan-2-yl)-2-thia-6,12,15-triazaoctadecan-4-yl]hexahydrofuro[3,2-d][1,2]oxazole-3-carboxamide (three-letter code: GHJ) (formula: $C_{29}H_{53}N_5O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	A	1	93	29	51	5	7	1	0	0
2	B	1	93	29	51	5	7	1	0	0

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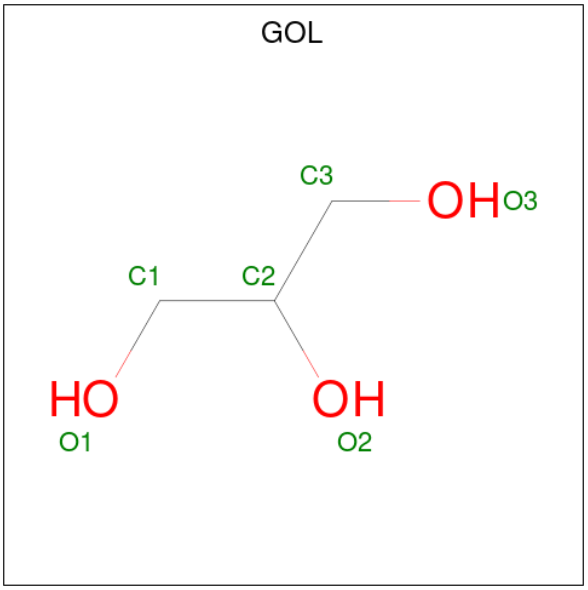
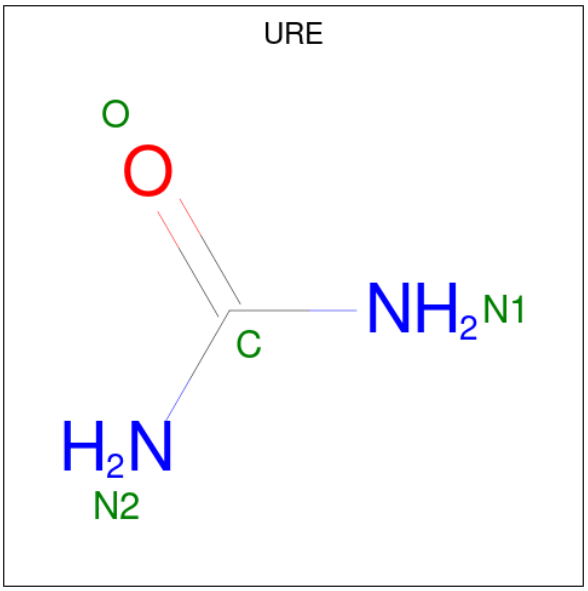
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	C	1	93	29	51	5	7	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



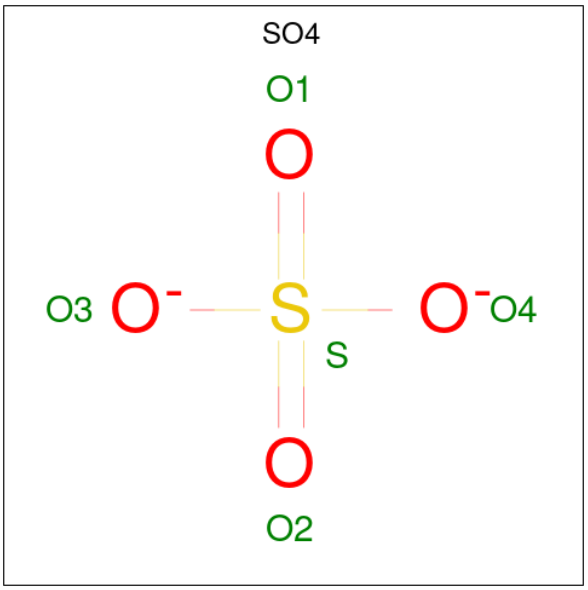
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C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

- Molecule 4 is UREA (three-letter code: URE) (formula: CH_4N_2O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	4	1	2	1	0	0
			Total	C	N	O		
4	A	1	4	1	2	1	0	0
			Total	C	N	O		
4	A	1	4	1	2	1	0	0
			Total	C	N	O		
4	B	1	4	1	2	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

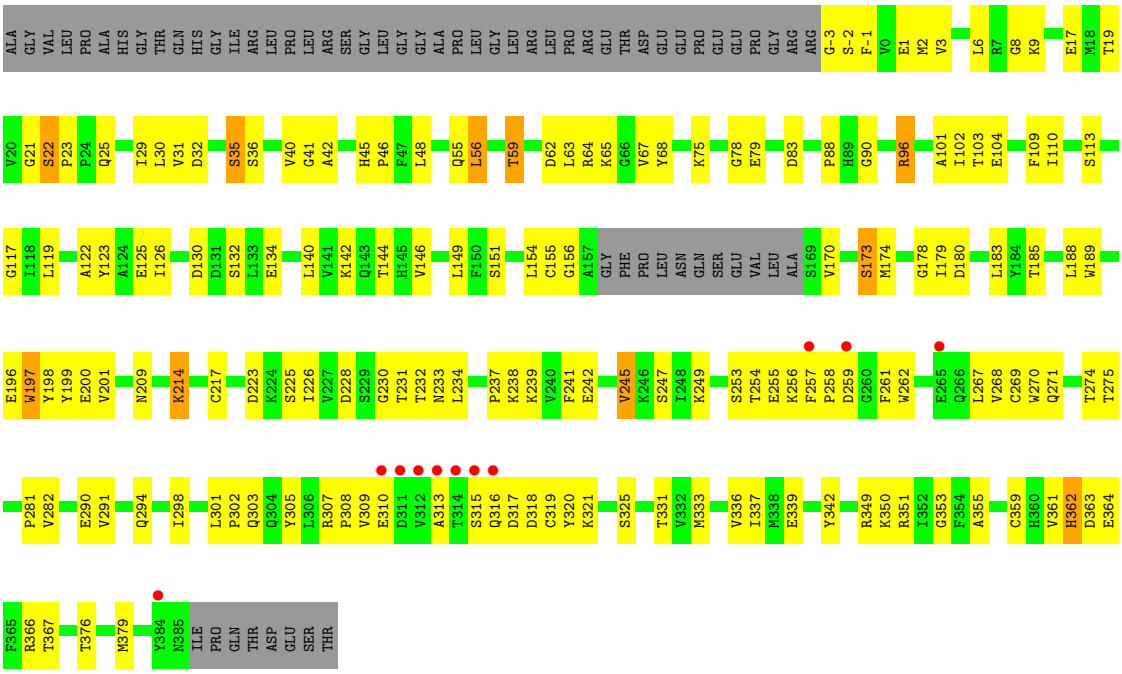
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	78	78	78	0	0
			Total	O		
6	B	82	82	82	0	0
			Total	O		
6	C	85	85	85	0	0

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.

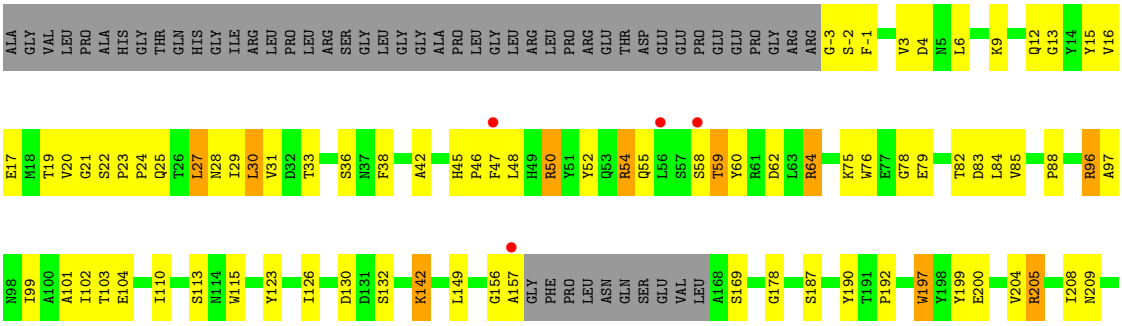
• Molecule 1: Beta-secretase 1

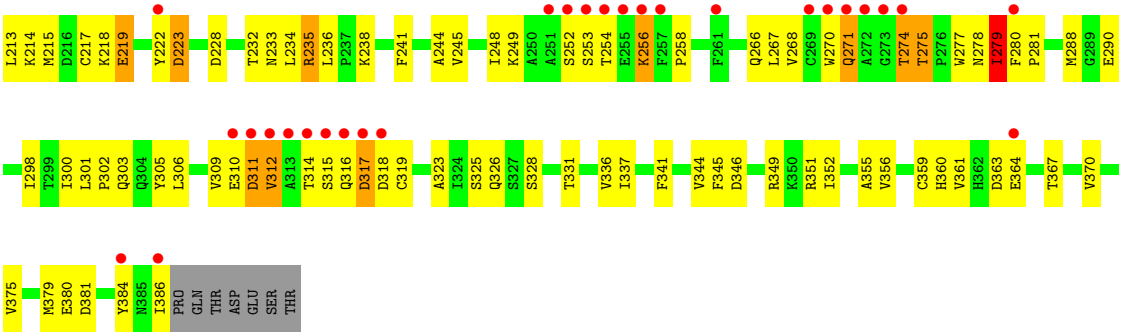
Chain A: 2% 49% 35% • 14%



• Molecule 1: Beta-secretase 1

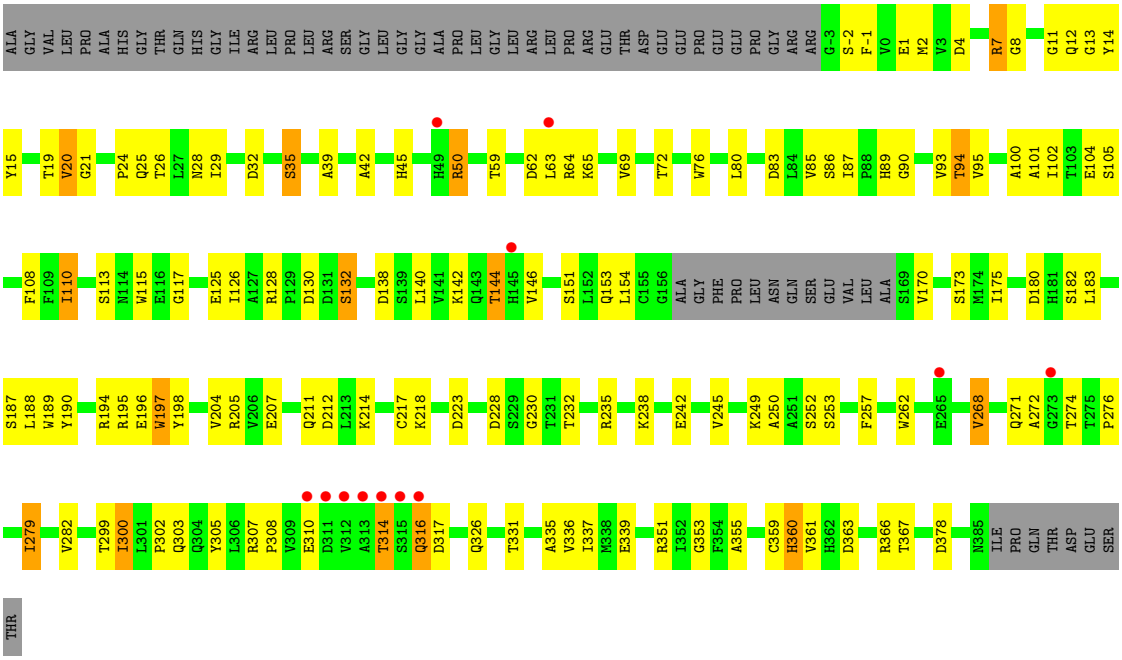
Chain B: 7% 49% 33% 5% 14%





- Molecule 1: Beta-secretase 1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.99Å 103.32Å 100.96Å 90.00° 102.98° 90.00°	Depositor
Resolution (Å)	40.30 – 2.85 40.30 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.30-2.85) 99.8 (40.30-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.172 , 0.218 0.174 , 0.219	Depositor DCC
R_{free} test set	1900 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9517	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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: GHJ, GOL, URE, SO4

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	0.35	0/3045	0.52	0/4138
1	B	0.37	1/3058 (0.0%)	0.52	0/4156
1	C	0.36	0/3040	0.53	0/4131
All	All	0.36	1/9143 (0.0%)	0.52	0/12425

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	279	ILE	C-N	6.07	1.48	1.34

There are no bond angle outliers.

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	2970	0	2881	114	0
1	B	2983	0	2897	146	1
1	C	2965	0	2876	110	1
2	A	42	51	0	4	0
2	B	42	51	0	1	0
2	C	42	51	0	3	0
3	A	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	24	3	0
3	C	18	0	24	13	0
4	A	12	0	12	1	0
4	B	4	0	4	0	0
5	C	5	0	0	0	0
6	A	78	0	0	1	0
6	B	82	0	0	4	0
6	C	85	0	0	6	0
All	All	9364	153	8742	372	1

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 21.

All (372) 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:A:267:LEU:HD11	1:A:309:VAL:HG21	1.25	1.18
1:B:82:THR:HG22	1:B:96:ARG:HH11	1.15	1.09
1:A:55:GLN:HG3	1:A:56:LEU:HD23	1.39	1.01
1:B:311:ASP:CB	1:B:314:THR:HB	1.92	0.98
1:C:95:VAL:HG11	1:C:140:LEU:HD12	1.47	0.95
1:B:271:GLN:O	1:B:274:THR:OG1	1.84	0.95
1:A:267:LEU:HD11	1:A:309:VAL:CG2	1.96	0.94
1:B:311:ASP:HB3	1:B:314:THR:HB	1.51	0.92
1:A:196:GLU:OE1	1:A:350:LYS:NZ	2.04	0.90
1:A:241:PHE:O	1:A:245:VAL:HG23	1.72	0.90
1:B:252:SER:HB2	1:B:279:ILE:HG23	1.52	0.89
1:B:82:THR:HG22	1:B:96:ARG:NH1	1.88	0.89
1:B:208:ILE:HD12	1:B:213:LEU:HD11	1.52	0.89
1:B:234:LEU:HD22	1:B:337:ILE:HD11	1.53	0.88
1:A:232:THR:O	1:A:336:VAL:HG13	1.75	0.85
1:B:323:ALA:HB1	1:B:336:VAL:HG21	1.59	0.84
1:C:110:ILE:HD11	1:C:115:TRP:CZ2	2.12	0.84
1:B:54:ARG:HD2	1:B:60:TYR:CE1	2.13	0.83
1:A:59:THR:O	1:A:96:ARG:NH2	2.12	0.83
1:C:272:ALA:HB2	1:C:316:GLN:O	1.79	0.82
1:A:55:GLN:HG3	1:A:56:LEU:CD2	2.11	0.81
1:A:156:GLY:O	1:A:170:VAL:HG23	1.81	0.81
1:C:130:ASP:OD1	1:C:132:SER:HB2	1.81	0.81
1:A:228:ASP:OD2	1:A:231:THR:OG1	1.98	0.81
1:A:363:ASP:OD1	1:A:364:GLU:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TYR:OH	1:C:339:GLU:OE1	2.00	0.80
1:C:276:PRO:HB2	1:C:279:ILE:HG12	1.63	0.80
1:B:245:VAL:O	1:B:249:LYS:HG2	1.81	0.79
1:B:241:PHE:O	1:B:245:VAL:HG23	1.81	0.79
1:B:192:PRO:HG2	1:B:288:MET:HE3	1.67	0.77
1:A:62:ASP:OD1	1:A:64:ARG:N	2.14	0.77
1:B:59:THR:HG21	1:B:84:LEU:CD1	2.15	0.77
1:B:244:ALA:O	1:B:248:ILE:HG13	1.84	0.77
1:C:271:GLN:O	1:C:274:THR:HB	1.85	0.76
1:B:233:ASN:ND2	1:B:325:SER:OG	2.18	0.75
1:B:192:PRO:HG2	1:B:288:MET:CE	2.16	0.75
1:C:282:VAL:CG1	1:C:299:THR:HG23	2.16	0.75
1:B:310:GLU:HG2	1:B:312:VAL:HG23	1.67	0.74
1:C:45:HIS:HE2	3:C:404:GOL:H2	1.52	0.74
1:C:108:PHE:H	3:C:404:GOL:H32	1.54	0.73
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.69	0.73
1:C:32:ASP:OD1	1:C:230:GLY:HA3	1.88	0.73
1:B:110:ILE:HB	1:B:113:SER:HB2	1.71	0.72
1:A:267:LEU:CD1	1:A:309:VAL:HG21	2.13	0.72
1:B:209:ASN:HB2	1:B:281:PRO:HB3	1.70	0.72
1:B:218:LYS:HE3	1:B:381:ASP:O	1.89	0.71
1:C:13:GLY:H	3:C:402:GOL:H32	1.54	0.71
1:A:238:LYS:O	1:A:242:GLU:HG3	1.91	0.71
1:A:110:ILE:HD11	2:A:401:GHJ:O42	1.90	0.71
1:B:204:VAL:O	1:B:205:ARG:HG2	1.92	0.70
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.74	0.70
1:B:271:GLN:N	1:B:274:THR:OG1	2.25	0.69
1:C:62:ASP:OD1	1:C:64:ARG:N	2.22	0.69
1:B:157:ALA:HB3	1:B:361:VAL:HG21	1.73	0.69
1:B:267:LEU:CD2	1:B:309:VAL:HG21	2.22	0.69
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.75	0.68
1:B:45:HIS:HB3	1:B:48:LEU:HD22	1.76	0.68
1:A:234:LEU:HD22	1:A:337:ILE:HD11	1.75	0.67
1:B:279:ILE:HG22	1:B:280:PHE:CD2	2.29	0.67
1:B:270:TRP:HB3	1:B:274:THR:CB	2.25	0.67
1:C:276:PRO:O	1:C:279:ILE:HG13	1.94	0.66
1:A:8:GLY:C	1:A:170:VAL:HG12	2.15	0.66
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.30	0.66
1:C:144:THR:OG1	1:C:146:VAL:HG23	1.94	0.66
1:A:29:ILE:HD12	1:A:117:GLY:HA3	1.78	0.66
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:TRP:HB3	1:B:274:THR:HB	1.78	0.66
1:A:301:LEU:HD12	1:A:361:VAL:CG2	2.26	0.66
1:B:82:THR:CG2	1:B:96:ARG:HG2	2.26	0.65
1:A:134:GLU:OE2	1:A:142:LYS:HD2	1.96	0.65
1:C:282:VAL:HG11	1:C:299:THR:HG23	1.77	0.65
1:B:204:VAL:C	1:B:205:ARG:HG2	2.16	0.65
1:C:11:GLY:H	3:C:402:GOL:H12	1.61	0.65
1:C:211:GLN:HG3	6:C:538:HOH:O	1.96	0.65
1:B:82:THR:CG2	1:B:96:ARG:HH11	2.00	0.65
1:C:8:GLY:C	1:C:170:VAL:HG22	2.17	0.65
1:B:311:ASP:HB2	1:B:314:THR:HB	1.77	0.65
1:B:267:LEU:HD21	1:B:309:VAL:HG21	1.80	0.64
1:B:54:ARG:HB3	1:B:60:TYR:CD1	2.32	0.64
1:A:55:GLN:CG	1:A:56:LEU:HD23	2.22	0.64
1:A:130:ASP:OD1	1:A:132:SER:CB	2.45	0.64
1:B:209:ASN:HA	6:B:509:HOH:O	1.97	0.64
1:C:238:LYS:HG3	1:C:326:GLN:OE1	1.98	0.64
1:A:307:ARG:HH21	1:A:321:LYS:HE2	1.64	0.63
1:A:17:GLU:HG2	1:A:88:PRO:HG2	1.81	0.63
1:A:48:LEU:HD21	1:A:109:PHE:CD1	2.34	0.63
1:A:32:ASP:OD1	1:A:35:SER:HB3	1.98	0.63
1:A:130:ASP:OD1	1:A:132:SER:HB3	1.99	0.63
1:B:82:THR:HG23	1:B:96:ARG:HG2	1.80	0.63
1:C:26:THR:HG22	1:C:50:ARG:HH21	1.63	0.63
1:B:55:GLN:OE1	1:B:55:GLN:N	2.22	0.62
1:A:155:CYS:O	1:A:170:VAL:HG22	1.99	0.62
1:A:271:GLN:O	1:A:274:THR:HB	1.98	0.62
1:C:45:HIS:NE2	3:C:404:GOL:H2	2.14	0.62
1:C:125:GLU:OE2	1:C:195:ARG:NH2	2.19	0.62
1:C:32:ASP:OD2	1:C:35:SER:OG	2.17	0.61
1:A:268:VAL:O	1:A:319:CYS:HA	2.00	0.61
1:A:274:THR:HG22	1:A:274:THR:O	1.99	0.61
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.31	0.61
1:C:108:PHE:N	3:C:404:GOL:H32	2.15	0.61
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.81	0.61
1:B:126:ILE:HG23	1:B:197:TRP:HB2	1.83	0.61
1:A:309:VAL:HG23	1:A:309:VAL:O	2.00	0.61
1:B:59:THR:HG21	1:B:84:LEU:HD11	1.82	0.61
1:C:335:ALA:O	1:C:339:GLU:HG3	2.00	0.61
1:A:36:SER:OG	1:A:123:TYR:O	2.14	0.61
1:B:270:TRP:HB3	1:B:274:THR:OG1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:TYR:OH	1:B:83:ASP:OD2	2.14	0.60
1:C:110:ILE:HD11	1:C:115:TRP:HZ2	1.65	0.60
1:A:255:GLU:O	1:A:256:LYS:HD3	2.01	0.60
1:A:269:CYS:HA	1:A:318:ASP:O	2.01	0.60
1:C:35:SER:HB3	2:C:401:GHJ:C36	2.32	0.60
1:B:245:VAL:HG12	1:B:249:LYS:HE3	1.84	0.60
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.84	0.60
1:C:108:PHE:H	3:C:404:GOL:C3	2.14	0.59
1:B:59:THR:HG21	1:B:84:LEU:HD12	1.84	0.59
1:A:180:ASP:HB3	1:A:183:LEU:HD12	1.84	0.59
1:C:13:GLY:N	3:C:402:GOL:H32	2.17	0.59
1:C:282:VAL:HG11	1:C:299:THR:CG2	2.31	0.59
1:A:140:LEU:HD11	1:A:146:VAL:HG21	1.83	0.59
1:A:259:ASP:N	1:A:259:ASP:OD1	2.34	0.59
1:B:238:LYS:HG2	1:B:326:GLN:OE1	2.03	0.59
1:B:302:PRO:HA	1:B:305:TYR:CE2	2.38	0.59
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.33	0.58
1:B:359:CYS:SG	1:B:359:CYS:O	2.61	0.58
1:C:245:VAL:CG1	1:C:249:LYS:HE3	2.34	0.58
1:C:86:SER:OG	1:C:94:THR:HB	2.04	0.58
1:A:307:ARG:NH2	1:A:321:LYS:HE2	2.19	0.58
1:C:26:THR:HG22	1:C:50:ARG:NH2	2.19	0.58
1:A:188:LEU:HD23	1:A:355:ALA:HB2	1.85	0.57
1:B:110:ILE:HD12	1:B:115:TRP:CZ2	2.39	0.57
1:C:271:GLN:HA	1:C:317:ASP:OD1	2.04	0.57
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.33	0.57
1:B:126:ILE:CG2	1:B:197:TRP:HB2	2.35	0.57
1:B:298:ILE:HG22	1:B:370:VAL:HG12	1.87	0.57
1:C:20:VAL:CG1	1:C:85:VAL:HG22	2.34	0.57
1:A:313:ALA:HB3	1:A:315:SER:O	2.04	0.57
1:B:126:ILE:HD12	2:B:401:GHJ:C36	2.34	0.57
1:B:252:SER:HB3	1:B:279:ILE:O	2.04	0.57
1:B:310:GLU:HG2	1:B:312:VAL:CG2	2.35	0.57
1:C:110:ILE:HD12	6:C:509:HOH:O	2.04	0.57
1:B:380:GLU:HA	1:B:380:GLU:OE1	2.04	0.56
1:C:303:GLN:CB	1:C:361:VAL:HG21	2.35	0.56
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.39	0.56
1:A:189:TRP:O	1:A:353:GLY:HA2	2.06	0.56
1:A:255:GLU:C	1:A:256:LYS:HD3	2.26	0.56
1:B:78:GLY:HA2	1:B:103:THR:HG23	1.86	0.56
1:C:11:GLY:N	3:C:402:GOL:H31	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLY:HA3	1:A:101:ALA:O	2.06	0.56
1:C:180:ASP:HB3	1:C:183:LEU:HD12	1.87	0.56
1:C:303:GLN:OE1	1:C:303:GLN:N	2.37	0.56
1:C:8:GLY:O	1:C:170:VAL:HG22	2.05	0.56
1:C:302:PRO:HA	1:C:305:TYR:CE2	2.41	0.56
1:C:359:CYS:O	1:C:359:CYS:SG	2.65	0.55
1:B:17:GLU:O	1:B:88:PRO:HD2	2.06	0.55
1:A:110:ILE:HB	1:A:113:SER:HB3	1.89	0.55
1:A:154:LEU:O	1:A:339:GLU:HA	2.07	0.55
1:B:33:THR:OG1	1:B:228:ASP:HA	2.07	0.55
1:C:95:VAL:CG1	1:C:140:LEU:HD12	2.29	0.55
1:A:316:GLN:O	1:A:317:ASP:HB2	2.06	0.55
1:C:314:THR:O	1:C:314:THR:HG22	2.07	0.55
1:A:41:GLY:HA2	1:A:102:ILE:HB	1.89	0.54
1:A:301:LEU:HD12	1:A:361:VAL:HG21	1.88	0.54
1:C:110:ILE:HD13	1:C:113:SER:HB3	1.89	0.54
1:C:250:ALA:O	1:C:253:SER:OG	2.25	0.54
1:B:323:ALA:CB	1:B:336:VAL:HG21	2.35	0.54
1:C:76:TRP:HB2	1:C:102:ILE:HG23	1.90	0.54
1:A:32:ASP:OD2	1:A:230:GLY:HA3	2.07	0.54
1:B:59:THR:HG22	1:B:96:ARG:HH21	1.73	0.54
1:B:270:TRP:O	1:B:317:ASP:HB3	2.07	0.54
1:C:204:VAL:O	3:C:403:GOL:O2	2.25	0.54
1:C:235:ARG:O	1:C:331:THR:HA	2.07	0.54
1:C:238:LYS:O	1:C:242:GLU:HG3	2.08	0.54
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.73	0.53
1:C:249:LYS:HE2	1:C:262:TRP:CD1	2.43	0.53
1:B:-3:GLY:O	1:B:-1:PHE:N	2.34	0.53
1:A:-3:GLY:HA3	1:A:-2:SER:HB2	1.89	0.53
1:A:307:ARG:O	1:A:320:TYR:HA	2.08	0.53
1:B:59:THR:HG22	1:B:96:ARG:NH2	2.23	0.53
1:B:142:LYS:HD3	1:B:142:LYS:N	2.24	0.53
1:B:13:GLY:HA3	1:B:30:LEU:HD11	1.90	0.53
1:B:252:SER:CB	1:B:279:ILE:HG23	2.33	0.53
1:C:153:GLN:OE1	1:C:183:LEU:HD22	2.09	0.52
1:C:-1:PHE:HB3	1:C:175:ILE:HG23	1.91	0.52
1:C:76:TRP:HA	1:C:105:SER:HA	1.91	0.52
1:B:62:ASP:OD1	1:B:64:ARG:N	2.36	0.52
1:A:302:PRO:HA	1:A:305:TYR:CE2	2.45	0.52
1:A:113:SER:OG	6:A:501:HOH:O	2.18	0.52
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.26	0.51
1:B:23:PRO:O	6:B:501:HOH:O	2.19	0.51
1:A:301:LEU:HD12	1:A:361:VAL:HG23	1.92	0.51
1:B:288:MET:HE1	6:B:568:HOH:O	2.09	0.51
1:A:258:PRO:O	1:A:261:PHE:HB3	2.11	0.51
1:A:376:THR:HG22	1:A:379:MET:HG2	1.91	0.51
1:C:19:THR:HA	1:C:25:GLN:O	2.11	0.51
1:C:360:HIS:O	1:C:360:HIS:ND1	2.44	0.51
1:B:130:ASP:OD1	1:B:132:SER:CB	2.59	0.51
1:B:267:LEU:HD23	1:B:309:VAL:HG21	1.93	0.51
1:C:110:ILE:CD1	1:C:115:TRP:CZ2	2.90	0.51
1:B:15:TYR:CD1	1:B:28:ASN:HB3	2.46	0.50
1:C:11:GLY:H	3:C:402:GOL:C1	2.23	0.50
1:B:215:MET:HE2	1:B:219:GLU:HB3	1.92	0.50
1:C:4:ASP:OD2	1:C:7:ARG:NH2	2.44	0.50
1:A:126:ILE:HG23	1:A:197:TRP:HB2	1.93	0.50
2:A:401:GHJ:O40	2:A:401:GHJ:C10	2.59	0.50
1:C:42:ALA:HB2	1:C:101:ALA:HB1	1.92	0.50
1:B:309:VAL:C	1:B:311:ASP:H	2.14	0.50
1:C:232:THR:O	1:C:336:VAL:HG13	2.12	0.50
1:C:8:GLY:HA2	1:C:15:TYR:CE2	2.46	0.50
1:C:363:ASP:HB3	1:C:366:ARG:O	2.12	0.50
1:A:239:LYS:HB2	1:A:239:LYS:NZ	2.25	0.50
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.46	0.50
1:B:204:VAL:HG11	1:B:379:MET:HG2	1.94	0.50
1:B:258:PRO:HB2	1:B:266:GLN:OE1	2.12	0.50
1:B:31:VAL:HG23	1:B:31:VAL:O	2.11	0.49
1:B:254:THR:OG1	1:B:279:ILE:HD11	2.12	0.49
1:B:268:VAL:O	1:B:319:CYS:HA	2.12	0.49
1:B:316:GLN:O	1:B:316:GLN:HG2	2.12	0.49
1:A:103:THR:C	1:A:104:GLU:HG3	2.33	0.49
1:B:76:TRP:HB2	1:B:102:ILE:HG23	1.93	0.49
1:B:271:GLN:C	1:B:274:THR:OG1	2.50	0.49
1:C:257:PHE:CD1	1:C:268:VAL:HG21	2.48	0.49
1:B:97:ALA:O	1:B:99:ILE:HG13	2.13	0.49
1:C:12:GLN:H	3:C:402:GOL:H31	1.76	0.49
1:A:307:ARG:HG3	1:A:308:PRO:HD2	1.95	0.49
1:A:363:ASP:HB3	1:A:366:ARG:O	2.12	0.49
1:B:192:PRO:HG2	1:B:288:MET:HE2	1.92	0.49
1:C:274:THR:CG2	1:C:274:THR:O	2.60	0.48
1:A:156:GLY:C	1:A:170:VAL:HG23	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:HA	1:B:23:PRO:C	2.33	0.48
1:B:75:LYS:HD2	6:C:508:HOH:O	2.13	0.48
1:A:233:ASN:ND2	1:A:325:SER:OG	2.33	0.48
1:A:29:ILE:HG21	1:A:119:LEU:HB2	1.95	0.48
1:C:69:VAL:HG22	1:C:128:ARG:HG3	1.95	0.48
1:C:180:ASP:OD1	1:C:182:SER:OG	2.23	0.48
1:B:113:SER:OG	1:B:115:TRP:CD1	2.66	0.48
1:B:234:LEU:HB2	1:B:337:ILE:HG12	1.96	0.48
1:B:310:GLU:HG2	1:B:310:GLU:O	2.13	0.48
1:C:212:ASP:OD1	1:C:214:LYS:N	2.35	0.48
1:A:301:LEU:HB3	1:A:303:GLN:OE1	2.14	0.48
1:B:349:ARG:HH22	3:B:404:GOL:C1	2.27	0.48
1:B:54:ARG:HD2	1:B:60:TYR:CZ	2.48	0.48
1:C:39:ALA:HB2	1:C:100:ALA:HB3	1.96	0.48
1:B:110:ILE:HD12	1:B:115:TRP:HZ2	1.77	0.48
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.49	0.48
1:B:355:ALA:HA	1:B:370:VAL:HG21	1.96	0.48
1:B:19:THR:HA	1:B:25:GLN:O	2.14	0.47
1:C:110:ILE:CD1	1:C:113:SER:HB3	2.44	0.47
1:B:3:VAL:O	1:B:4:ASP:HB2	2.12	0.47
1:B:301:LEU:HD11	1:B:367:THR:CA	2.44	0.47
1:C:190:TYR:CG	1:C:351:ARG:HD2	2.49	0.47
1:A:36:SER:OG	1:A:126:ILE:HG13	2.14	0.47
1:A:42:ALA:HB2	1:A:101:ALA:HB1	1.96	0.47
1:A:290:GLU:OE1	1:A:351:ARG:NH1	2.46	0.47
1:C:274:THR:O	1:C:274:THR:HG22	2.14	0.47
1:B:351:ARG:HH22	3:B:404:GOL:H31	1.79	0.47
1:C:126:ILE:HG23	1:C:197:TRP:HB2	1.97	0.47
1:B:33:THR:HG21	1:B:345:PHE:CZ	2.49	0.47
1:A:359:CYS:O	1:A:359:CYS:SG	2.73	0.47
1:A:-1:PHE:CZ	1:A:178:GLY:HA3	2.49	0.47
1:A:185:THR:HB	4:A:405:URE:O	2.14	0.47
1:C:110:ILE:HD12	1:C:110:ILE:H	1.80	0.47
1:C:238:LYS:HE2	1:C:242:GLU:OE2	2.14	0.46
1:B:277:TRP:HZ3	1:B:306:LEU:HD12	1.79	0.46
1:A:19:THR:HA	1:A:25:GLN:O	2.15	0.46
1:A:268:VAL:HG11	1:A:270:TRP:CH2	2.51	0.46
1:B:54:ARG:HH11	1:B:54:ARG:CG	2.29	0.46
1:C:21:GLY:HA2	1:C:83:ASP:OD2	2.16	0.46
1:A:259:ASP:HA	1:A:262:TRP:HD1	1.80	0.46
1:B:113:SER:OG	1:B:115:TRP:NE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLY:O	1:C:24:PRO:HA	2.14	0.46
1:B:27:LEU:HA	1:B:50:ARG:NH1	2.31	0.46
1:B:45:HIS:CB	1:B:48:LEU:HD22	2.45	0.46
1:B:222:TYR:O	1:B:223:ASP:CB	2.64	0.46
1:B:309:VAL:C	1:B:311:ASP:N	2.69	0.46
1:A:249:LYS:HE2	1:A:262:TRP:CD1	2.51	0.46
1:C:29:ILE:HD12	1:C:117:GLY:HA3	1.97	0.46
1:A:22:SER:HA	1:A:23:PRO:C	2.36	0.45
1:B:54:ARG:HB3	1:B:60:TYR:CE1	2.51	0.45
1:A:214:LYS:HE3	1:A:214:LYS:O	2.16	0.45
1:A:274:THR:O	1:A:274:THR:CG2	2.63	0.45
1:B:190:TYR:HB2	1:B:290:GLU:CD	2.36	0.45
1:C:104:GLU:OE2	6:C:501:HOH:O	2.21	0.45
1:A:301:LEU:HD13	1:A:363:ASP:HB2	1.99	0.45
1:B:149:LEU:HD23	1:B:178:GLY:HA2	1.97	0.45
1:B:215:MET:HE2	1:B:215:MET:HB3	1.84	0.45
1:C:282:VAL:CG1	1:C:299:THR:CG2	2.90	0.45
1:A:201:VAL:HG21	1:A:333:MET:CE	2.47	0.45
1:A:237:PRO:HD3	1:A:331:THR:OG1	2.17	0.45
1:B:6:LEU:CD2	1:B:16:VAL:HB	2.47	0.45
1:B:270:TRP:O	1:B:318:ASP:N	2.39	0.45
1:C:207:GLU:HA	1:C:211:GLN:O	2.16	0.45
1:A:40:VAL:O	1:A:102:ILE:HG13	2.17	0.45
1:B:156:GLY:O	1:B:157:ALA:HB2	2.16	0.45
1:A:282:VAL:HG12	1:A:301:LEU:HD23	1.99	0.45
1:C:110:ILE:HD13	1:C:113:SER:CB	2.47	0.45
1:C:189:TRP:O	1:C:353:GLY:HA2	2.17	0.45
1:C:194:ARG:NH1	6:C:503:HOH:O	2.50	0.45
1:B:310:GLU:OE2	1:B:312:VAL:HG21	2.16	0.44
1:B:363:ASP:OD1	1:B:363:ASP:N	2.39	0.44
1:C:87:ILE:HG22	1:C:90:GLY:N	2.32	0.44
1:C:314:THR:O	1:C:314:THR:CG2	2.65	0.44
1:B:55:GLN:H	1:B:55:GLN:CD	2.11	0.44
1:A:110:ILE:CD1	2:A:401:GHJ:O42	2.63	0.44
2:A:401:GHJ:O39	2:A:401:GHJ:S11	2.76	0.44
1:A:48:LEU:HD21	1:A:109:PHE:CE1	2.53	0.44
1:B:79:GLU:HG2	6:B:563:HOH:O	2.17	0.44
1:C:72:THR:HB	2:C:401:GHJ:O39	2.17	0.44
1:C:154:LEU:O	1:C:339:GLU:HA	2.17	0.44
1:A:31:VAL:HG23	1:A:31:VAL:O	2.17	0.44
1:A:241:PHE:O	1:A:245:VAL:CG2	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLY:HA2	1:A:83:ASP:OD1	2.18	0.44
1:A:197:TRP:HD1	1:A:197:TRP:H	1.66	0.44
1:C:205:ARG:HG3	3:C:403:GOL:H2	1.99	0.44
1:A:361:VAL:HG23	1:A:362:HIS:N	2.33	0.43
1:B:315:SER:O	1:B:316:GLN:HB3	2.18	0.43
1:A:199:TYR:O	1:A:226:ILE:HA	2.18	0.43
1:A:6:LEU:HD21	1:A:174:MET:HB2	2.01	0.43
1:A:270:TRP:CE3	1:A:275:THR:HG23	2.54	0.43
1:C:-1:PHE:HA	1:C:2:MET:HE3	2.00	0.43
1:B:298:ILE:HB	1:B:341:PHE:CZ	2.54	0.43
1:B:311:ASP:HB3	1:B:314:THR:CB	2.37	0.43
1:A:122:ALA:CB	1:A:126:ILE:HD11	2.49	0.43
1:A:197:TRP:CG	1:A:198:TYR:N	2.86	0.43
1:B:36:SER:OG	1:B:123:TYR:O	2.28	0.43
1:B:204:VAL:O	1:B:205:ARG:CG	2.66	0.43
1:B:281:PRO:O	1:B:305:TYR:OH	2.26	0.43
1:A:201:VAL:O	1:A:225:SER:HB2	2.18	0.42
1:C:300:ILE:HD13	1:C:337:ILE:CD1	2.49	0.42
1:A:144:THR:OG1	1:A:146:VAL:HG23	2.18	0.42
1:B:29:ILE:HG21	1:B:38:PHE:HE1	1.85	0.42
1:B:204:VAL:HA	1:B:217:CYS:SG	2.60	0.42
1:A:179:ILE:HG23	1:A:342:TYR:CE2	2.52	0.42
1:B:130:ASP:OD1	1:B:132:SER:HB2	2.20	0.42
1:B:384:TYR:HE1	1:B:386:ILE:HB	1.85	0.42
1:A:45:HIS:HB3	1:A:48:LEU:HG	2.02	0.42
1:B:208:ILE:CD1	1:B:213:LEU:HD11	2.38	0.41
1:A:241:PHE:CE2	1:A:245:VAL:HG21	2.55	0.41
1:C:196:GLU:OE2	6:C:502:HOH:O	2.21	0.41
1:C:307:ARG:HA	1:C:308:PRO:HD3	1.94	0.41
1:B:370:VAL:O	1:B:370:VAL:HG23	2.21	0.41
1:A:67:VAL:HG22	1:A:68:TYR:N	2.35	0.41
1:A:214:LYS:HD2	1:A:214:LYS:HA	1.73	0.41
1:B:235:ARG:O	1:B:331:THR:HA	2.21	0.41
1:C:197:TRP:CG	1:C:198:TYR:N	2.87	0.41
1:B:302:PRO:HG2	1:B:303:GLN:OE1	2.21	0.41
1:C:28:ASN:O	1:C:29:ILE:HD13	2.20	0.41
1:C:93:VAL:HG21	1:C:140:LEU:HD11	2.02	0.41
1:C:228:ASP:OD2	2:C:401:GHJ:O21	2.39	0.41
1:A:349:ARG:HE	1:A:349:ARG:HB3	1.70	0.41
1:C:63:LEU:HD12	1:C:80:LEU:HB3	2.02	0.41
1:A:3:VAL:HA	1:A:173:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PHE:N	1:B:47:PHE:CD1	2.89	0.41
1:B:149:LEU:HD11	1:B:344:VAL:HG13	2.03	0.41
1:B:197:TRP:CD1	1:B:197:TRP:N	2.89	0.41
1:B:375:VAL:O	3:B:402:GOL:H32	2.20	0.41
1:C:2:MET:HG2	1:C:89:HIS:O	2.20	0.41
1:C:12:GLN:OE1	1:C:113:SER:HA	2.21	0.41
1:C:204:VAL:HA	1:C:217:CYS:SG	2.61	0.41
1:B:21:GLY:O	1:B:24:PRO:HA	2.22	0.41
1:A:122:ALA:HB3	1:A:126:ILE:HD11	2.03	0.40
1:C:300:ILE:O	1:C:300:ILE:HG13	2.14	0.40
1:B:9:LYS:HB2	1:B:12:GLN:HB2	2.04	0.40
1:B:209:ASN:HB2	1:B:281:PRO:CB	2.46	0.40
1:B:256:LYS:HD2	1:B:256:LYS:C	2.42	0.40
1:A:350:LYS:HE2	1:A:350:LYS:HB2	1.64	0.40
1:B:323:ALA:HB1	1:B:336:VAL:CG2	2.39	0.40
1:B:346:ASP:HB3	1:B:351:ARG:HG3	2.03	0.40
1:C:197:TRP:HD1	1:C:197:TRP:H	1.68	0.40
1:A:291:VAL:CG2	1:A:294:GLN:CB	2.99	0.40
1:B:300:ILE:HD13	1:B:337:ILE:HD13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:NH2	1:C:378:ASP:OD2[1_455]	2.06	0.14

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	374/441 (85%)	360 (96%)	13 (4%)	1 (0%)	41 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	376/441 (85%)	357 (95%)	16 (4%)	3 (1%)	19	46
1	C	373/441 (85%)	362 (97%)	10 (3%)	1 (0%)	41	68
All	All	1123/1323 (85%)	1079 (96%)	39 (4%)	5 (0%)	34	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-2	SER
1	B	223	ASP
1	A	223	ASP
1	C	223	ASP
1	B	312	VAL

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	322/372 (87%)	293 (91%)	29 (9%)	9	25
1	B	323/372 (87%)	290 (90%)	33 (10%)	7	20
1	C	322/372 (87%)	294 (91%)	28 (9%)	10	27
All	All	967/1116 (87%)	877 (91%)	90 (9%)	9	24

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	9	LYS
1	A	22	SER
1	A	30	LEU
1	A	35	SER
1	A	56	LEU
1	A	59	THR
1	A	63	LEU
1	A	65	LYS

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Mol	Chain	Res	Type
1	A	75	LYS
1	A	79	GLU
1	A	96	ARG
1	A	125	GLU
1	A	149	LEU
1	A	151	SER
1	A	173	SER
1	A	197	TRP
1	A	200	GLU
1	A	214	LYS
1	A	217	CYS
1	A	245	VAL
1	A	247	SER
1	A	253	SER
1	A	254	THR
1	A	257	PHE
1	A	298	ILE
1	A	310	GLU
1	A	362	HIS
1	A	367	THR
1	B	27	LEU
1	B	30	LEU
1	B	50	ARG
1	B	54	ARG
1	B	58	SER
1	B	59	THR
1	B	64	ARG
1	B	96	ARG
1	B	104	GLU
1	B	142	LYS
1	B	169	SER
1	B	187	SER
1	B	197	TRP
1	B	200	GLU
1	B	205	ARG
1	B	214	LYS
1	B	219	GLU
1	B	232	THR
1	B	235	ARG
1	B	236	LEU
1	B	253	SER
1	B	256	LYS

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Mol	Chain	Res	Type
1	B	271	GLN
1	B	274	THR
1	B	275	THR
1	B	278	ASN
1	B	279	ILE
1	B	311	ASP
1	B	317	ASP
1	B	328	SER
1	B	356	VAL
1	B	360	HIS
1	B	364	GLU
1	C	-2	SER
1	C	1	GLU
1	C	7	ARG
1	C	20	VAL
1	C	35	SER
1	C	50	ARG
1	C	59	THR
1	C	65	LYS
1	C	94	THR
1	C	110	ILE
1	C	132	SER
1	C	138	ASP
1	C	142	LYS
1	C	144	THR
1	C	151	SER
1	C	173	SER
1	C	187	SER
1	C	197	TRP
1	C	218	LYS
1	C	252	SER
1	C	268	VAL
1	C	279	ILE
1	C	300	ILE
1	C	310	GLU
1	C	314	THR
1	C	316	GLN
1	C	360	HIS
1	C	367	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	GLN
1	B	233	ASN
1	B	271	GLN
1	C	316	GLN

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)

17 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	$\#\|Z\| > 2$
2	GHJ	B	401	-	41,43,43	3.96	15 (36%)	50,59,59	1.56	10 (20%)
3	GOL	B	402	-	5,5,5	0.38	0	5,5,5	0.40	0
3	GOL	A	404	-	5,5,5	0.29	0	5,5,5	0.40	0
3	GOL	A	403	-	5,5,5	0.32	0	5,5,5	0.38	0
4	URE	A	405	-	3,3,3	3.66	2 (66%)	3,3,3	0.66	0
3	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.25	0
3	GOL	C	402	-	5,5,5	0.31	0	5,5,5	0.33	0
4	URE	B	405	-	3,3,3	3.58	2 (66%)	3,3,3	0.72	0
2	GHJ	C	401	-	41,43,43	3.93	14 (34%)	50,59,59	2.10	13 (26%)
2	GHJ	A	401	-	41,43,43	4.17	16 (39%)	50,59,59	2.80	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	URE	A	407	-	3,3,3	3.70	2 (66%)	3,3,3	0.52	0
4	URE	A	406	-	3,3,3	3.69	2 (66%)	3,3,3	0.85	0
3	GOL	A	402	-	5,5,5	0.32	0	5,5,5	0.40	0
5	SO4	C	405	-	4,4,4	0.15	0	6,6,6	0.14	0
3	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	C	403	-	5,5,5	0.41	0	5,5,5	0.33	0
3	GOL	C	404	-	5,5,5	0.35	0	5,5,5	0.41	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
2	GHJ	B	401	-	-	11/52/71/71	0/2/2/2
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-
2	GHJ	C	401	-	-	22/52/71/71	0/2/2/2
2	GHJ	A	401	-	1/1/19/20	21/52/71/71	0/2/2/2
3	GOL	A	402	-	-	2/4/4/4	-
3	GOL	B	404	-	-	1/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	C	404	-	-	4/4/4/4	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GHJ	C01-C05	-15.00	1.29	1.52
2	B	401	GHJ	C01-C05	-13.98	1.31	1.52
2	C	401	GHJ	C01-C05	-13.59	1.32	1.52
2	A	401	GHJ	C05-C06	-10.84	1.35	1.54
2	B	401	GHJ	C05-C06	-10.70	1.36	1.54
2	C	401	GHJ	C05-C06	-9.85	1.37	1.54
2	A	401	GHJ	C13-N14	8.73	1.53	1.34
2	C	401	GHJ	C13-N14	8.30	1.52	1.34
2	B	401	GHJ	C13-N14	7.55	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GHJ	C07-N08	7.01	1.49	1.34
2	C	401	GHJ	C07-N08	6.98	1.49	1.34
2	C	401	GHJ	O02-C01	6.79	1.55	1.41
2	B	401	GHJ	C07-N08	6.70	1.48	1.34
2	A	401	GHJ	O02-C01	6.69	1.55	1.41
2	B	401	GHJ	O02-C01	6.68	1.55	1.41
2	B	401	GHJ	C24-N25	6.67	1.48	1.34
2	C	401	GHJ	C24-N25	6.65	1.48	1.34
2	A	401	GHJ	C24-N25	6.54	1.48	1.34
2	C	401	GHJ	C04-C03	-5.98	1.35	1.51
2	B	401	GHJ	C04-C03	-5.86	1.35	1.51
2	B	401	GHJ	C27-N28	5.84	1.46	1.33
2	A	401	GHJ	C27-N28	5.83	1.46	1.33
2	A	401	GHJ	C04-C03	-5.80	1.35	1.51
2	C	401	GHJ	C27-N28	5.27	1.45	1.33
4	A	406	URE	C-N1	4.39	1.46	1.34
4	A	407	URE	C-N1	4.39	1.46	1.34
4	A	405	URE	C-N2	4.36	1.46	1.34
4	A	407	URE	C-N2	4.34	1.46	1.34
4	A	406	URE	C-N2	4.31	1.46	1.34
2	A	401	GHJ	C06-N41	-4.25	1.37	1.46
4	A	405	URE	C-N1	4.24	1.45	1.34
4	B	405	URE	C-N2	4.21	1.45	1.34
4	B	405	URE	C-N1	4.18	1.45	1.34
2	B	401	GHJ	C06-N41	-4.03	1.37	1.46
2	C	401	GHJ	C06-N41	-4.02	1.37	1.46
2	A	401	GHJ	O02-C03	3.01	1.51	1.42
2	A	401	GHJ	O40-C07	-3.01	1.17	1.23
2	A	401	GHJ	O39-C13	-3.01	1.17	1.23
2	B	401	GHJ	O02-C03	2.83	1.51	1.42
2	C	401	GHJ	O02-C03	2.75	1.51	1.42
2	B	401	GHJ	O39-C13	-2.66	1.18	1.23
2	C	401	GHJ	O40-C07	-2.66	1.18	1.23
2	C	401	GHJ	O39-C13	-2.65	1.18	1.23
2	A	401	GHJ	O33-C27	-2.59	1.18	1.23
2	A	401	GHJ	O21-C20	-2.52	1.38	1.43
2	C	401	GHJ	O21-C20	-2.51	1.38	1.43
2	B	401	GHJ	O40-C07	-2.49	1.18	1.23
2	A	401	GHJ	C15-N14	2.40	1.50	1.46
2	C	401	GHJ	O33-C27	-2.38	1.18	1.23
2	B	401	GHJ	O21-C20	-2.31	1.38	1.43
2	A	401	GHJ	O37-C24	-2.21	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GHJ	C26-N25	-2.09	1.41	1.45
2	B	401	GHJ	O33-C27	-2.07	1.19	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	GHJ	C15-N14-C13	8.00	137.21	123.07
2	A	401	GHJ	C09-C13-N14	7.99	134.22	116.70
2	A	401	GHJ	O39-C13-N14	-6.68	110.56	122.93
2	A	401	GHJ	C26-C27-N28	6.23	127.16	116.41
2	C	401	GHJ	C09-C13-N14	5.46	128.68	116.70
2	C	401	GHJ	C26-C27-N28	5.38	125.69	116.41
2	A	401	GHJ	C09-C10-S11	5.08	122.27	114.04
2	C	401	GHJ	C15-N14-C13	4.75	131.47	123.07
2	A	401	GHJ	C16-C15-N14	4.36	115.83	110.18
2	C	401	GHJ	C03-C04-C05	4.16	109.16	103.32
2	A	401	GHJ	O02-C01-C05	-4.16	101.05	107.05
2	C	401	GHJ	C23-C24-N25	3.84	120.53	116.42
2	C	401	GHJ	O39-C13-N14	-3.84	115.83	122.93
2	B	401	GHJ	C16-C15-N14	-3.80	105.27	110.18
2	A	401	GHJ	C23-C24-N25	3.49	120.16	116.42
2	B	401	GHJ	C34-C26-C27	-3.47	102.70	111.38
2	C	401	GHJ	O33-C27-N28	-3.44	115.60	122.99
2	A	401	GHJ	C10-C09-N08	-3.43	101.72	111.00
2	B	401	GHJ	C09-C10-S11	-3.42	108.51	114.04
2	A	401	GHJ	O33-C27-N28	-3.34	115.81	122.99
2	A	401	GHJ	C12-S11-C10	3.30	107.36	101.30
2	C	401	GHJ	C01-C05-C06	3.18	107.94	102.19
2	B	401	GHJ	C03-C04-C05	3.11	107.69	103.32
2	B	401	GHJ	C23-C22-C20	-3.05	109.34	114.74
2	B	401	GHJ	C04-C05-C01	3.00	106.25	102.34
2	C	401	GHJ	C04-C05-C01	2.92	106.14	102.34
2	B	401	GHJ	C13-C09-N08	-2.76	103.66	111.16
2	B	401	GHJ	C17-C16-C15	-2.72	110.44	115.84
2	A	401	GHJ	C10-C09-C13	2.66	115.50	109.73
2	A	401	GHJ	C23-C22-C20	-2.63	110.08	114.74
2	C	401	GHJ	C16-C15-C20	2.61	116.50	112.55
2	A	401	GHJ	O39-C13-C09	-2.50	115.19	120.45
2	C	401	GHJ	O39-C13-C09	-2.37	115.47	120.45
2	C	401	GHJ	C12-S11-C10	2.35	105.62	101.30
2	B	401	GHJ	C23-C24-N25	2.34	118.93	116.42
2	A	401	GHJ	O40-C07-C06	-2.33	115.92	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	GHJ	C06-C07-N08	2.28	121.41	116.48
2	A	401	GHJ	C30-C29-N28	-2.21	106.34	113.72
2	B	401	GHJ	C15-N14-C13	-2.18	119.23	123.07
2	C	401	GHJ	C27-C26-N25	-2.12	104.60	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	GHJ	C06

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GHJ	C13-C09-C10-S11
2	A	401	GHJ	C09-C10-S11-C12
2	A	401	GHJ	C16-C15-N14-C13
2	A	401	GHJ	C16-C15-C20-O21
2	A	401	GHJ	C16-C15-C20-C22
2	A	401	GHJ	N14-C15-C20-O21
2	A	401	GHJ	N14-C15-C20-C22
2	A	401	GHJ	C20-C22-C23-C24
2	B	401	GHJ	N41-C06-C07-O40
2	B	401	GHJ	N41-C06-C07-N08
2	B	401	GHJ	C20-C22-C23-C24
2	B	401	GHJ	C27-C26-C34-C36
2	C	401	GHJ	N41-C06-C07-O40
2	C	401	GHJ	N41-C06-C07-N08
2	C	401	GHJ	C16-C15-N14-C13
2	C	401	GHJ	C16-C15-C20-O21
2	C	401	GHJ	C16-C15-C20-C22
2	C	401	GHJ	N14-C15-C20-O21
2	C	401	GHJ	N14-C15-C20-C22
2	C	401	GHJ	C20-C22-C23-C38
2	C	401	GHJ	C20-C22-C23-C24
3	A	402	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-C3
3	A	404	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	C	404	GOL	O1-C1-C2-C3
3	C	404	GOL	C1-C2-C3-O3
3	C	404	GOL	O2-C2-C3-O3
2	B	401	GHJ	N25-C26-C34-C35

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Mol	Chain	Res	Type	Atoms
2	B	401	GHJ	C27-C26-C34-C35
2	B	401	GHJ	N25-C26-C34-C36
2	A	401	GHJ	O33-C27-N28-C29
2	C	401	GHJ	O33-C27-N28-C29
2	A	401	GHJ	C26-C27-N28-C29
2	C	401	GHJ	C26-C27-N28-C29
2	C	401	GHJ	N28-C29-C30-C31
3	A	403	GOL	O1-C1-C2-O2
2	C	401	GHJ	C15-C16-C17-C19
2	C	401	GHJ	O39-C13-N14-C15
2	A	401	GHJ	O39-C13-N14-C15
2	C	401	GHJ	C09-C13-N14-C15
2	A	401	GHJ	C09-C13-N14-C15
2	A	401	GHJ	C15-C16-C17-C18
2	C	401	GHJ	C15-C16-C17-C18
3	B	403	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
2	A	401	GHJ	C10-C09-N08-C07
3	B	403	GOL	O1-C1-C2-O2
3	C	404	GOL	O1-C1-C2-O2
2	A	401	GHJ	N08-C09-C10-S11
3	A	402	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O1-C1-C2-C3
2	A	401	GHJ	N41-C06-C07-O40
2	C	401	GHJ	C10-C09-N08-C07
2	A	401	GHJ	N41-C06-C07-N08
2	C	401	GHJ	C13-C09-N08-C07
2	B	401	GHJ	C09-C10-S11-C12
2	A	401	GHJ	C15-C16-C17-C19
2	C	401	GHJ	N28-C29-C30-C32
2	A	401	GHJ	C13-C09-N08-C07
2	C	401	GHJ	N08-C09-C10-S11
2	C	401	GHJ	N08-C09-C13-O39
3	B	402	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
2	B	401	GHJ	C20-C22-C23-C38
2	C	401	GHJ	N08-C09-C13-N14
3	B	403	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-C3
2	A	401	GHJ	N08-C09-C13-N14
2	A	401	GHJ	N08-C09-C13-O39

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Mol	Chain	Res	Type	Atoms
2	B	401	GHJ	N08-C09-C13-O39
2	B	401	GHJ	C10-C09-C13-O39

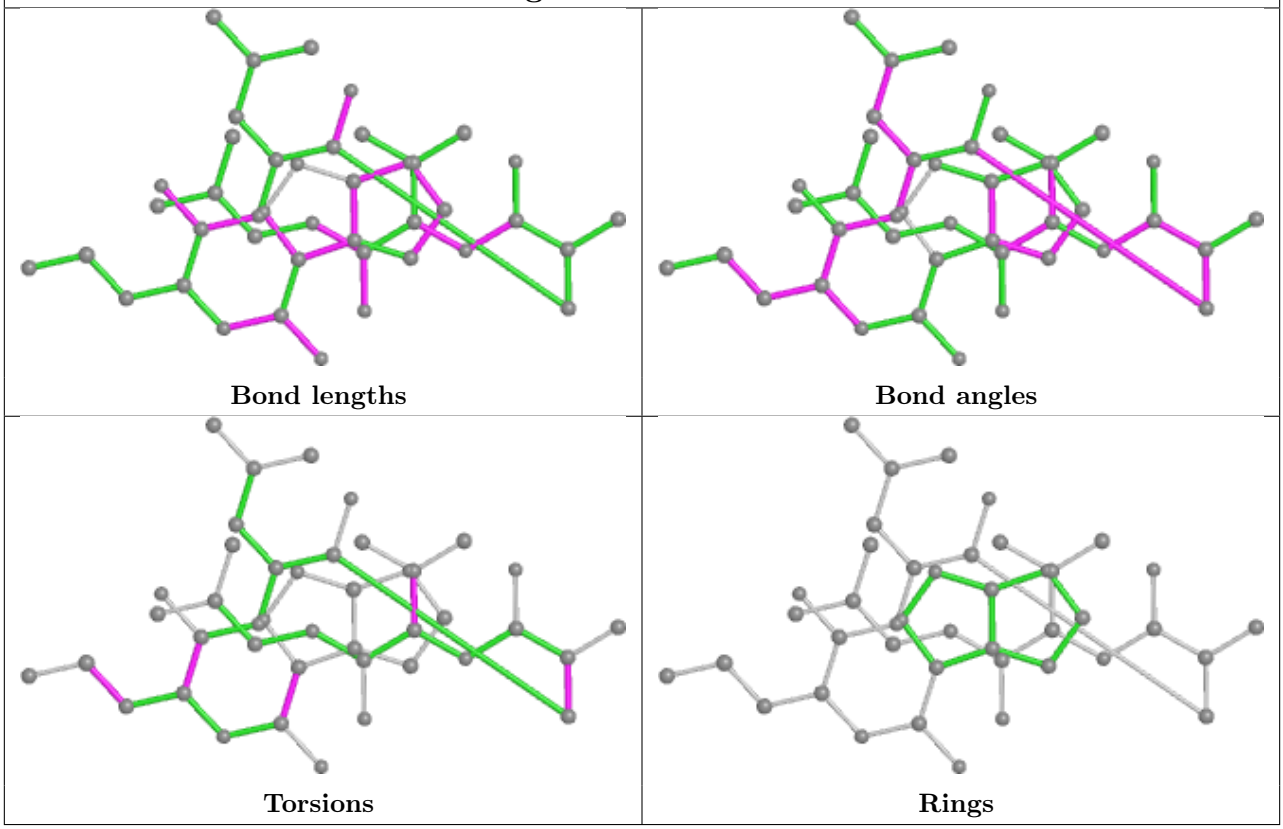
There are no ring outliers.

9 monomers are involved in 25 short contacts:

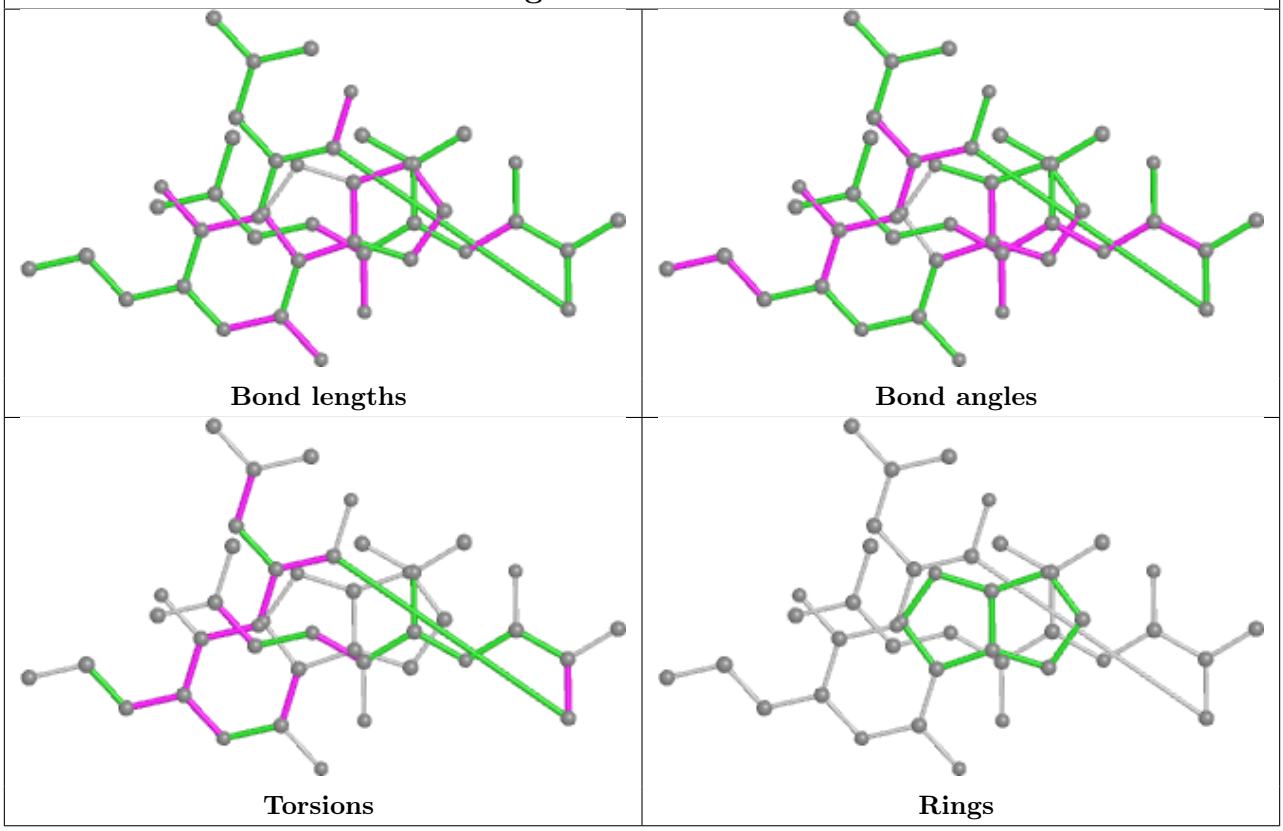
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GHJ	1	0
3	B	402	GOL	1	0
4	A	405	URE	1	0
3	C	402	GOL	6	0
2	C	401	GHJ	3	0
2	A	401	GHJ	4	0
3	B	404	GOL	2	0
3	C	403	GOL	2	0
3	C	404	GOL	5	0

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.

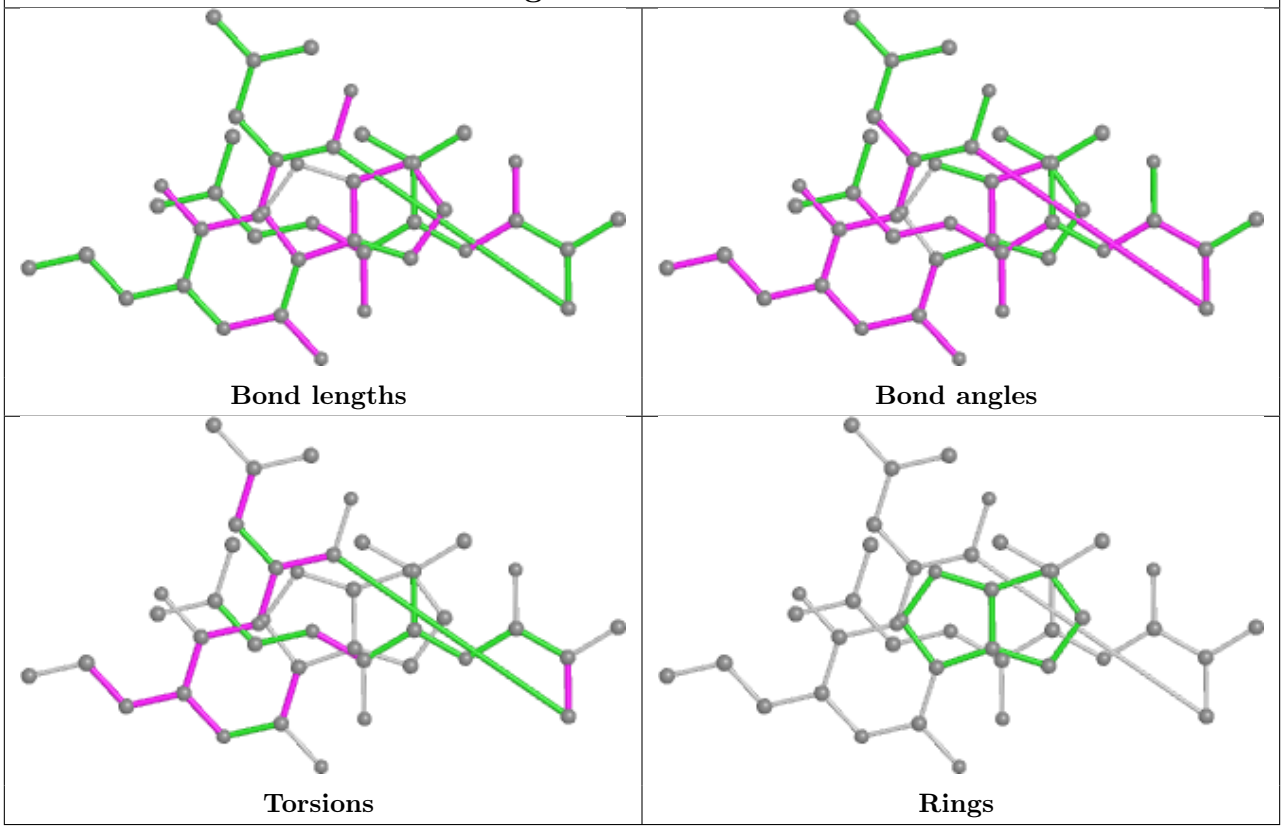
Ligand GHJ B 401



Ligand GHJ C 401



Ligand GHJ A 401



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	378/441 (85%)	0.02	11 (2%)	51	47	35, 55, 81, 134	0
1	B	380/441 (86%)	0.24	32 (8%)	11	7	35, 58, 104, 128	0
1	C	377/441 (85%)	0.04	12 (3%)	47	42	39, 54, 79, 121	0
All	All	1135/1323 (85%)	0.10	55 (4%)	30	26	35, 55, 92, 134	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	312	VAL	7.5
1	B	312	VAL	7.3
1	A	312	VAL	5.9
1	B	313	ALA	5.7
1	A	314	THR	5.4
1	A	315	SER	5.2
1	B	316	GLN	5.0
1	A	313	ALA	5.0
1	C	314	THR	4.6
1	C	310	GLU	4.6
1	B	254	THR	4.6
1	C	316	GLN	4.3
1	C	313	ALA	4.1
1	B	311	ASP	3.9
1	B	272	ALA	3.9
1	B	314	THR	3.8
1	B	310	GLU	3.8
1	B	255	GLU	3.7
1	C	311	ASP	3.7
1	B	252	SER	3.7
1	B	269	CYS	3.5
1	A	316	GLN	3.4
1	B	384	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	257	PHE	3.2
1	B	315	SER	3.2
1	C	145	HIS	3.1
1	B	256	LYS	3.1
1	A	311	ASP	3.0
1	A	310	GLU	2.9
1	C	265	GLU	2.9
1	B	280	PHE	2.9
1	A	265	GLU	2.9
1	B	318	ASP	2.8
1	B	317	ASP	2.7
1	B	261	PHE	2.7
1	B	253	SER	2.6
1	B	56	LEU	2.6
1	B	273	GLY	2.6
1	B	157	ALA	2.6
1	B	274	THR	2.5
1	A	259	ASP	2.5
1	B	386	ILE	2.4
1	C	273	GLY	2.4
1	B	364	GLU	2.3
1	B	270	TRP	2.3
1	B	222	TYR	2.3
1	B	58	SER	2.2
1	B	251	ALA	2.2
1	B	271	GLN	2.2
1	C	63	LEU	2.2
1	C	315	SER	2.2
1	C	49	HIS	2.1
1	A	384	TYR	2.1
1	A	257	PHE	2.0
1	B	47	PHE	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)

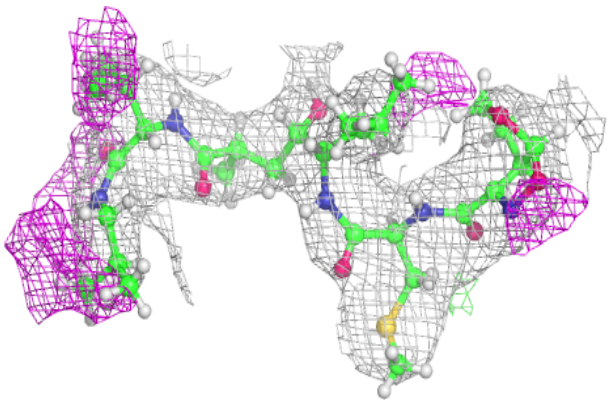
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

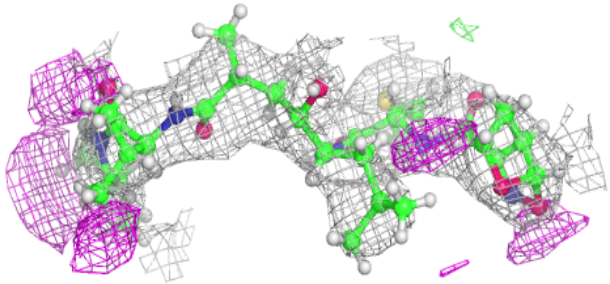
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	404	6/6	0.73	0.43	58,66,67,67	0
3	GOL	B	404	6/6	0.76	0.29	61,70,73,74	0
4	URE	A	405	4/4	0.78	0.27	64,69,72,73	0
4	URE	A	406	4/4	0.80	0.31	69,73,75,79	0
4	URE	A	407	4/4	0.81	0.25	72,74,81,82	0
3	GOL	B	403	6/6	0.86	0.21	60,66,67,68	0
3	GOL	A	402	6/6	0.86	0.18	48,58,61,62	0
5	SO4	C	405	5/5	0.86	0.20	93,97,112,119	0
3	GOL	C	403	6/6	0.90	0.23	57,61,65,66	0
3	GOL	B	402	6/6	0.90	0.20	54,58,62,63	0
3	GOL	A	403	6/6	0.91	0.12	77,81,83,85	0
3	GOL	C	402	6/6	0.91	0.17	59,60,66,66	0
2	GHJ	A	401	42/42	0.95	0.21	42,58,75,79	0
4	URE	B	405	4/4	0.95	0.23	50,63,65,67	0
2	GHJ	C	401	42/42	0.95	0.19	38,54,66,77	0
3	GOL	A	404	6/6	0.96	0.15	61,63,70,72	0
2	GHJ	B	401	42/42	0.96	0.20	43,58,74,85	0

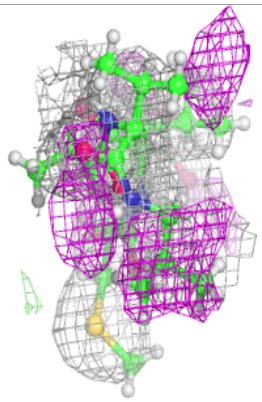
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GHJ A 401:

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

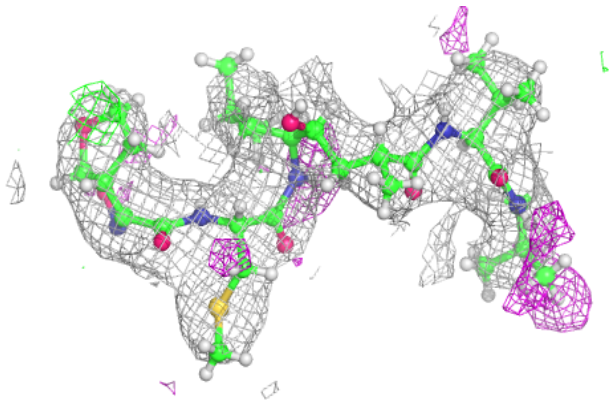


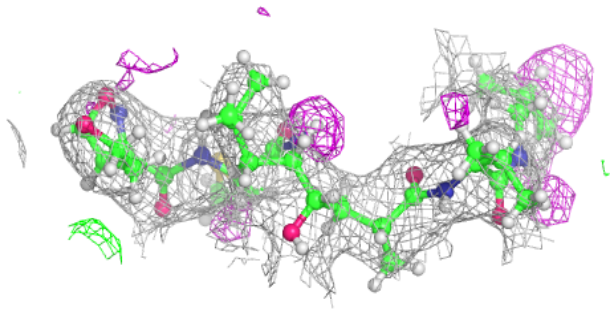


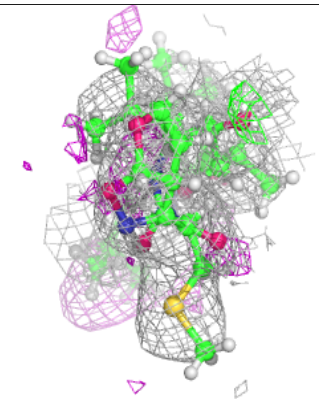


Electron density around GHJ C 401:

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

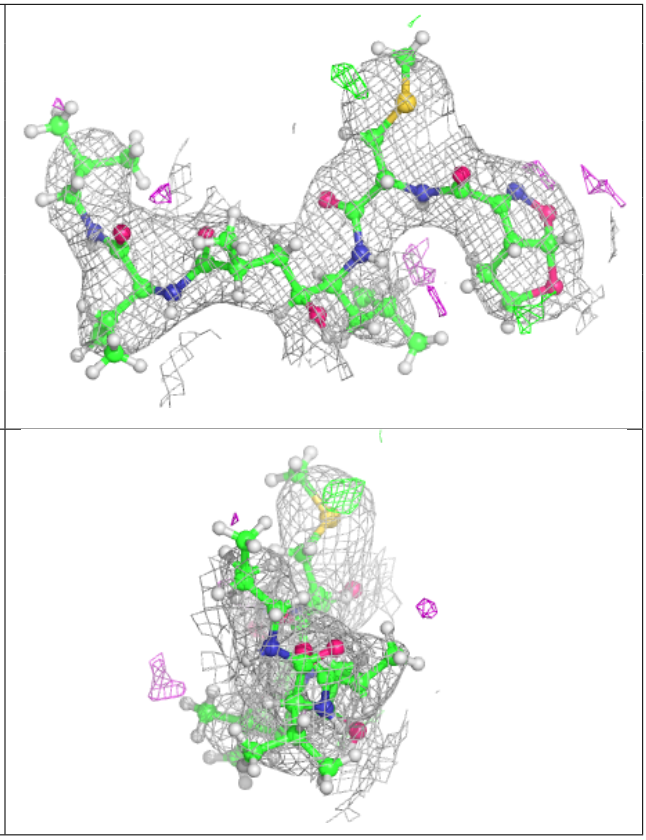






Electron density around GHJ B 401:

$2mF_o$-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.