Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:59 AM EDT

PDB ID	:	1OT7
Title	:	Structural Basis for 3-deoxy-CDCA Binding and Activation of FXR
Authors	:	Mi, L.Z.; Devarakonda, S.; Harp, J.M.; Han, Q.; Pellicciari, R.; Willson, T.M.; Khorasanizadeh, S.; Rastinejad, F.
Deposited on	:	2003-03-21
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

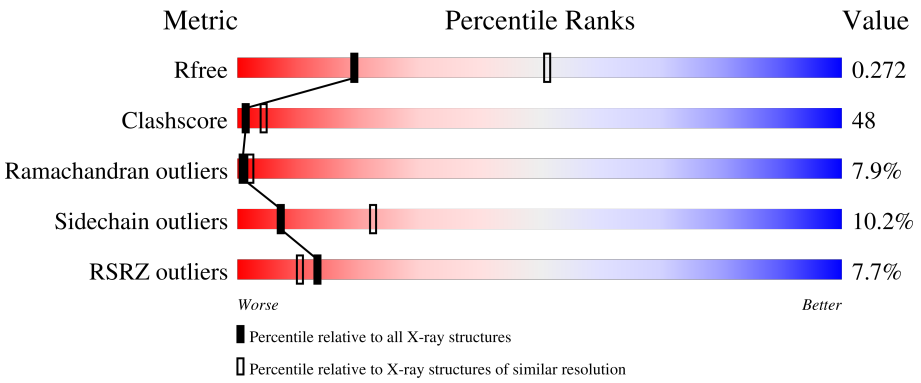
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	229	10%; 34%, 55%, 10% •
1	B	229	6%; 35%, 53%, 9% •
2	C	12	8%; 42%, 42%, 17%
2	D	12	42%, 42%, 17%
2	E	12	8%; 67%, 17%, 17%

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
4	IU5	B	1002	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4140 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.

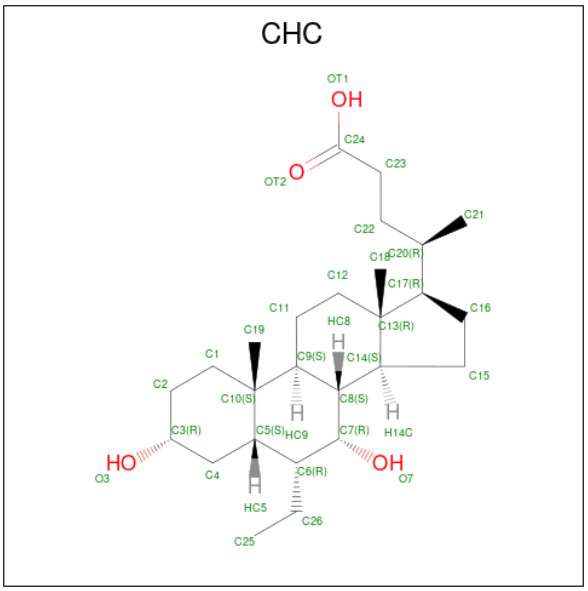
- Molecule 1 is a protein called Bile Acid Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1876	1201	311	353	11	0	0	0
1	B	229	1876	1201	311	353	11	0	0	0

- Molecule 2 is a protein called dodecamer peptide fragment of RPGR-interacting protein 1.

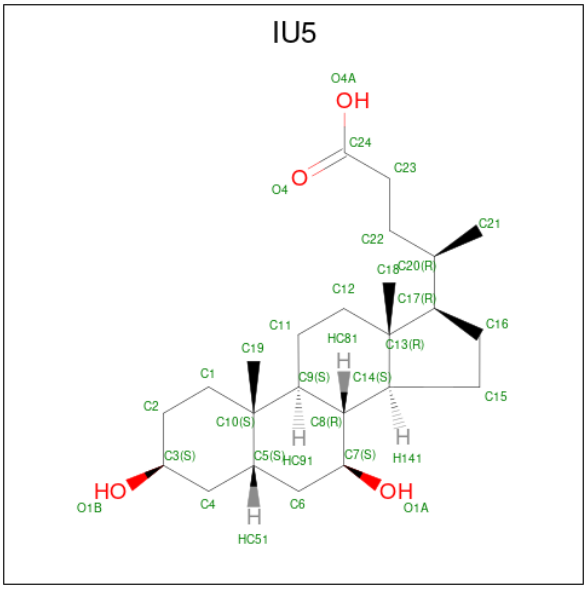
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	12	100	64	17	19	0	0	0
2	D	12	103	65	17	21	0	0	0
2	E	12	100	64	17	19	0	0	0

- Molecule 3 is 6-ETHYL-CHENODEOXYCHOLIC ACID (three-letter code: CHC) (formula: $C_{26}H_{44}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	30	26	4	0	0

- Molecule 4 is ISO-URSODEOXYCHOLIC ACID (three-letter code: IU5) (formula: $C_{24}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	27	24	3	0	0

- Molecule 5 is water.

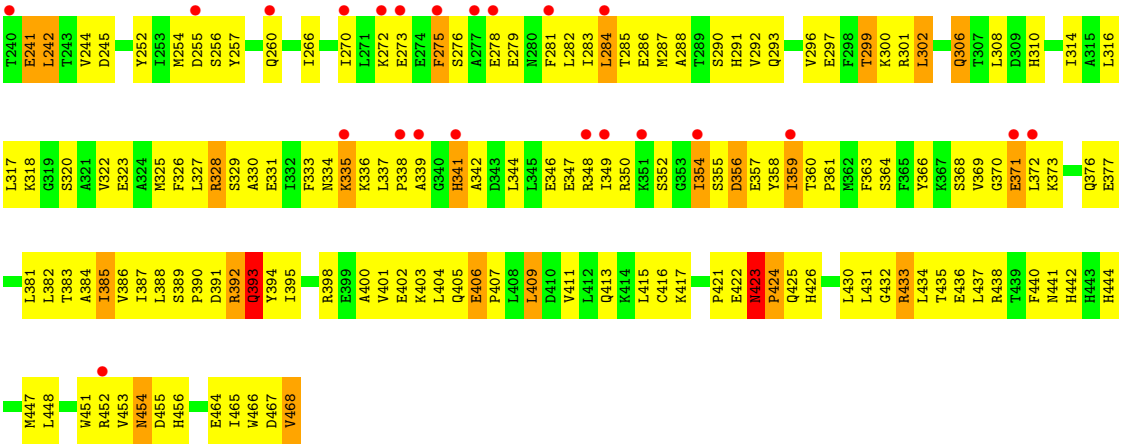
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	9	9	9	0	0
			Total	O		
5	B	16	16	16	0	0
			Total	O		
5	D	3	3	3	0	0

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.

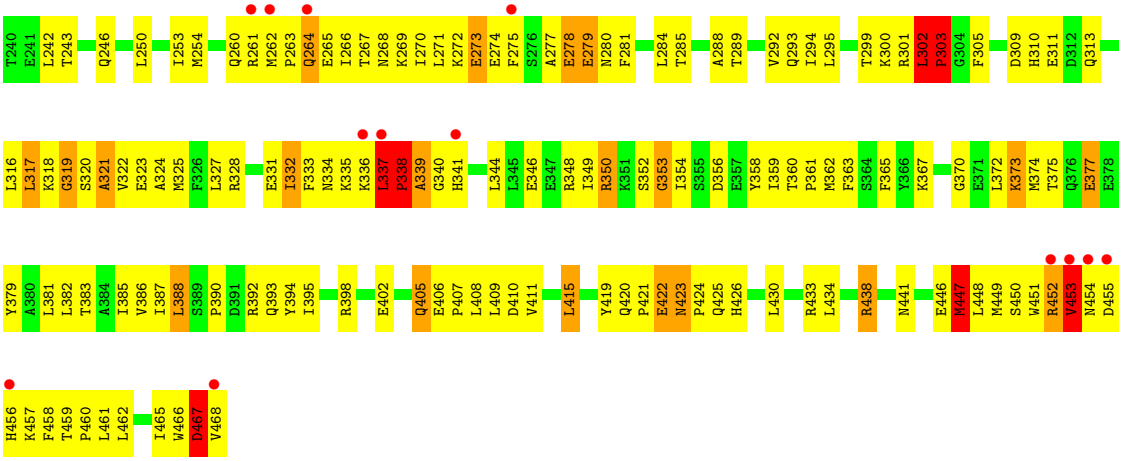
• Molecule 1: Bile Acid Receptor

Chain A:



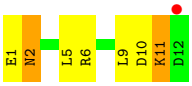
• Molecule 1: Bile Acid Receptor

Chain B:



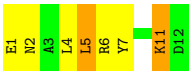
• Molecule 2: dodecamer peptide fragment of RPGR-interacting protein 1

Chain C:



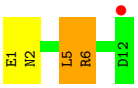
• Molecule 2: dodecamer peptide fragment of RPGR-interacting protein 1

Chain D:



• Molecule 2: dodecamer peptide fragment of RPGR-interacting protein 1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.54Å 107.13Å 69.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.90 49.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	75.4 (19.96-2.90) 98.1 (49.77-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.279 0.224 , 0.272	Depositor DCC
R_{free} test set	880 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4140	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: CHC, IU5

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	0.42	0/1913	0.72	1/2581 (0.0%)
1	B	0.45	0/1914	0.74	1/2584 (0.0%)
2	C	0.38	0/100	0.67	0/132
2	D	0.38	0/103	0.60	0/136
2	E	0.38	0/100	0.59	0/132
All	All	0.43	0/4130	0.73	2/5565 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	302	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	393	GLN	N-CA-C	5.12	124.83	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	1876	0	1875	177	0
1	B	1876	0	1876	212	0
2	C	100	0	104	6	0
2	D	103	0	106	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	100	0	104	9	0
3	A	30	0	43	3	0
4	B	27	0	37	4	0
5	A	9	0	0	1	0
5	B	16	0	0	10	0
5	D	3	0	0	0	0
All	All	4140	0	4145	399	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 48.

All (399) 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:B:262:MET:HG3	1:B:268:ASN:HD21	1.14	1.06
1:B:405:GLN:HE21	1:B:409:LEU:HD11	1.20	1.00
1:B:270:ILE:HG23	1:B:274:GLU:HG3	1.42	0.99
1:B:336:LYS:HG3	1:B:338:PRO:HD2	1.42	0.98
1:B:350:ARG:HB2	5:B:1:HOH:O	1.63	0.98
1:A:297:GLU:O	1:A:300:LYS:HG3	1.64	0.97
1:B:462:LEU:HA	1:B:465:ILE:HD11	1.49	0.95
1:B:383:THR:O	1:B:387:ILE:HG13	1.67	0.94
1:B:336:LYS:HE2	1:B:338:PRO:HB2	1.47	0.94
1:B:299:THR:HA	1:B:302:LEU:HD22	1.49	0.92
1:A:407:PRO:O	1:A:411:VAL:HG23	1.70	0.91
1:A:335:LYS:HE3	1:A:373:LYS:HA	1.50	0.90
1:A:306:GLN:HE21	1:A:306:GLN:N	1.70	0.88
1:B:332:ILE:O	1:B:335:LYS:HB2	1.74	0.88
1:B:374:MET:HB2	1:B:379:TYR:CE1	2.10	0.86
1:A:423:ASN:HB2	1:A:424:PRO:O	1.77	0.84
1:A:350:ARG:HD3	1:A:359:ILE:HD12	1.60	0.83
1:B:334:ASN:ND2	1:B:370:GLY:HA3	1.93	0.83
1:B:405:GLN:NE2	1:B:409:LEU:HD11	1.94	0.82
1:B:350:ARG:CD	5:B:1:HOH:O	2.27	0.82
1:A:241:GLU:H	1:A:241:GLU:CD	1.83	0.82
1:B:262:MET:CG	1:B:268:ASN:HD21	1.93	0.81
1:A:451:TRP:O	1:A:452:ARG:HA	1.79	0.81
1:B:263:PRO:O	1:B:264:GLN:HB2	1.79	0.81
1:B:426:HIS:CE1	1:B:430:LEU:HD21	2.15	0.81
1:B:318:LYS:NZ	2:D:2:ASN:HD21	1.79	0.81
1:B:253:ILE:HD12	1:B:254:MET:N	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ILE:HD13	1:B:409:LEU:HD23	1.62	0.80
1:B:466:TRP:O	1:B:467:ASP:HB2	1.81	0.79
1:B:350:ARG:CG	5:B:1:HOH:O	2.30	0.79
1:A:424:PRO:HG2	1:A:425:GLN:H	1.47	0.78
1:B:346:GLU:CG	5:B:15:HOH:O	2.31	0.78
1:B:447:MET:HE1	1:B:451:TRP:CE3	2.20	0.77
1:A:323:GLU:HB3	1:A:437:LEU:HD13	1.67	0.77
1:B:350:ARG:HD2	5:B:1:HOH:O	1.81	0.77
1:A:335:LYS:NZ	1:A:373:LYS:HG2	2.00	0.76
1:B:319:GLY:O	1:B:392:ARG:NH2	2.18	0.76
1:B:374:MET:HE3	1:B:430:LEU:HD22	1.67	0.76
1:B:350:ARG:CB	5:B:1:HOH:O	2.28	0.76
1:A:383:THR:HG22	1:A:387:ILE:CD1	2.16	0.75
1:A:381:LEU:O	1:A:385:ILE:HG23	1.87	0.74
1:B:299:THR:HA	1:B:302:LEU:CD2	2.17	0.74
1:A:424:PRO:C	1:A:426:HIS:H	1.90	0.73
1:A:278:GLU:HB2	1:A:456:HIS:NE2	2.04	0.72
1:A:383:THR:HG22	1:A:387:ILE:HD12	1.70	0.72
1:B:452:ARG:CZ	1:B:453:VAL:H	2.02	0.72
1:A:372:LEU:HD13	1:A:430:LEU:HD23	1.71	0.72
1:B:388:LEU:HD23	1:B:408:LEU:CD1	2.21	0.71
1:A:270:ILE:HD11	1:A:341:HIS:HB2	1.73	0.70
1:A:423:ASN:ND2	1:A:424:PRO:HA	2.06	0.70
1:A:292:VAL:O	1:A:296:VAL:HG23	1.91	0.70
1:A:306:GLN:HE21	1:A:306:GLN:H	1.40	0.70
1:A:423:ASN:HD22	1:A:424:PRO:HA	1.56	0.69
1:B:250:LEU:HD12	1:B:253:ILE:HD11	1.73	0.69
1:A:276:SER:HB2	1:A:279:GLU:HB3	1.75	0.69
1:A:354:ILE:HG12	1:A:447:MET:CE	2.22	0.69
1:B:272:LYS:HG2	1:B:344:LEU:HD23	1.74	0.69
1:B:289:THR:HG23	1:B:461:LEU:HD23	1.74	0.69
1:A:288:ALA:O	1:A:292:VAL:HG23	1.93	0.68
1:B:261:ARG:HA	1:B:261:ARG:HH11	1.58	0.68
1:B:336:LYS:HG3	1:B:338:PRO:CD	2.23	0.68
1:A:384:ALA:O	1:A:388:LEU:HD23	1.93	0.68
1:B:262:MET:HG3	1:B:268:ASN:ND2	1.98	0.67
1:A:411:VAL:O	1:A:415:LEU:HB2	1.94	0.67
1:A:316:LEU:O	1:A:320:SER:OG	2.12	0.67
1:A:334:ASN:ND2	1:A:370:GLY:HA2	2.08	0.67
1:B:270:ILE:HG23	1:B:274:GLU:CG	2.23	0.67
1:B:353:GLY:HA3	5:B:26:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:O	1:A:387:ILE:HD12	1.95	0.67
1:B:452:ARG:NE	1:B:453:VAL:H	1.93	0.67
1:A:423:ASN:HB2	1:A:424:PRO:C	2.14	0.66
1:B:420:GLN:N	1:B:421:PRO:HD3	2.09	0.66
1:B:462:LEU:HA	1:B:465:ILE:CD1	2.24	0.66
1:A:276:SER:HB2	1:A:279:GLU:CB	2.25	0.66
1:A:323:GLU:HB3	1:A:437:LEU:CD1	2.25	0.66
1:B:339:ALA:HB1	1:B:341:HIS:CE1	2.31	0.66
1:A:395:ILE:HD11	1:A:398:ARG:HG2	1.77	0.66
1:B:447:MET:HE3	1:B:447:MET:O	1.95	0.66
1:A:349:ILE:HG21	3:A:1001:CHC:H253	1.77	0.65
1:B:457:LYS:H	1:B:457:LYS:HD2	1.61	0.65
1:A:390:PRO:O	1:A:395:ILE:HD11	1.97	0.65
1:A:354:ILE:HD12	1:A:359:ILE:HG22	1.78	0.65
1:B:321:ALA:O	1:B:324:ALA:HB3	1.96	0.65
1:A:354:ILE:HG12	1:A:447:MET:HE1	1.79	0.65
1:B:263:PRO:HD2	1:B:294:ILE:HD11	1.79	0.65
1:A:400:ALA:O	1:A:404:LEU:HD13	1.98	0.64
1:A:451:TRP:C	1:A:452:ARG:HD3	2.17	0.64
1:B:375:THR:OG1	1:B:377:GLU:HG2	1.98	0.64
1:B:405:GLN:HA	1:B:408:LEU:HD12	1.80	0.63
1:A:282:LEU:HA	1:A:285:THR:HG22	1.79	0.63
1:A:281:PHE:O	1:A:285:THR:HG22	1.98	0.63
1:B:335:LYS:HG3	1:B:336:LYS:HG2	1.81	0.63
1:A:423:ASN:HB2	1:A:424:PRO:CA	2.27	0.63
1:A:405:GLN:HG2	1:A:409:LEU:HD22	1.80	0.63
1:A:292:VAL:HG21	1:A:465:ILE:HD11	1.81	0.62
1:B:292:VAL:CG1	1:B:461:LEU:HD21	2.29	0.62
1:A:382:LEU:O	1:A:386:VAL:HG23	2.00	0.62
1:B:268:ASN:O	1:B:271:LEU:HB3	1.98	0.62
1:B:407:PRO:O	1:B:411:VAL:HG23	2.00	0.61
1:A:350:ARG:HH11	1:A:359:ILE:HD11	1.65	0.61
1:A:426:HIS:O	1:A:430:LEU:HG	2.01	0.61
1:B:462:LEU:HD23	1:B:465:ILE:HD11	1.81	0.61
1:A:451:TRP:O	1:A:452:ARG:HD3	2.00	0.61
1:B:336:LYS:O	1:B:337:LEU:HB2	2.00	0.61
1:A:354:ILE:HD12	1:A:359:ILE:CG2	2.31	0.61
1:B:457:LYS:HD2	1:B:457:LYS:N	2.16	0.61
1:B:346:GLU:HG2	5:B:15:HOH:O	2.00	0.60
1:B:422:GLU:CD	1:B:422:GLU:H	2.04	0.60
1:B:292:VAL:O	1:B:295:LEU:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:OH	1:A:331:GLU:OE2	2.20	0.60
1:A:464:GLU:CD	2:C:2:ASN:HA	2.21	0.60
1:A:433:ARG:NH1	1:A:436:GLU:OE2	2.35	0.60
1:B:338:PRO:O	1:B:339:ALA:CB	2.50	0.60
1:B:453:VAL:O	1:B:453:VAL:HG13	2.02	0.60
1:A:275:PHE:O	1:A:279:GLU:HB3	2.02	0.60
1:B:242:LEU:HG	1:B:246:GLN:HB2	1.84	0.60
1:B:322:VAL:HG23	1:B:323:GLU:N	2.16	0.60
1:B:264:GLN:HE22	2:E:1:GLU:HB3	1.67	0.59
1:B:336:LYS:CG	1:B:338:PRO:HD2	2.27	0.59
1:B:272:LYS:HG2	1:B:344:LEU:CD2	2.32	0.59
1:A:292:VAL:HG11	1:A:465:ILE:HD13	1.84	0.59
1:B:277:ALA:O	1:B:280:ASN:ND2	2.34	0.59
1:B:266:ILE:O	1:B:270:ILE:HG13	2.03	0.59
1:A:325:MET:O	1:A:329:SER:OG	2.14	0.59
1:B:269:LYS:C	1:B:271:LEU:H	2.06	0.59
1:B:325:MET:HE1	4:B:1002:IU5:HC21	1.83	0.59
1:B:264:GLN:HE22	2:E:1:GLU:CB	2.16	0.59
1:B:271:LEU:O	1:B:271:LEU:HD13	2.03	0.59
1:A:296:VAL:HG12	1:A:296:VAL:O	2.03	0.58
1:B:325:MET:CE	4:B:1002:IU5:HC21	2.32	0.58
1:A:393:GLN:HG2	1:A:394:TYR:CE1	2.38	0.58
1:B:292:VAL:HG11	1:B:461:LEU:HD11	1.84	0.58
1:A:372:LEU:HD13	1:A:430:LEU:CD2	2.32	0.58
1:B:358:TYR:CD2	1:B:447:MET:HG3	2.38	0.58
1:A:283:ILE:HD12	1:A:348:ARG:HH21	1.69	0.57
1:B:393:GLN:O	1:B:394:TYR:HB2	2.04	0.57
1:B:405:GLN:HE21	1:B:409:LEU:CD1	2.05	0.57
1:A:350:ARG:HH11	1:A:359:ILE:CD1	2.16	0.57
1:A:348:ARG:O	1:A:352:SER:HB3	2.05	0.57
1:B:318:LYS:HZ2	2:D:2:ASN:HD21	1.53	0.57
1:A:241:GLU:O	1:A:242:LEU:CB	2.53	0.57
1:B:360:THR:N	1:B:361:PRO:HD2	2.20	0.57
1:B:269:LYS:C	1:B:271:LEU:N	2.57	0.57
1:A:444:HIS:HD2	3:A:1001:CHC:O3	1.87	0.56
1:B:299:THR:HG22	1:B:387:ILE:HD13	1.87	0.56
1:B:393:GLN:HG2	1:B:394:TYR:CD2	2.40	0.56
1:B:278:GLU:OE1	1:B:279:GLU:N	2.39	0.56
1:A:389:SER:HB2	1:A:392:ARG:HH11	1.69	0.56
1:B:458:PHE:CE1	1:B:468:VAL:HG21	2.41	0.56
1:B:328:ARG:NH2	1:B:331:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:HD21	1:B:370:GLY:HA3	1.69	0.55
2:D:6:ARG:HB3	2:D:6:ARG:NH1	2.21	0.55
1:A:292:VAL:HG21	1:A:465:ILE:CD1	2.37	0.55
1:B:336:LYS:O	1:B:337:LEU:CB	2.55	0.55
1:B:466:TRP:O	1:B:467:ASP:CB	2.52	0.55
2:E:6:ARG:HG3	2:E:6:ARG:HH11	1.71	0.55
1:A:358:TYR:CE1	1:A:447:MET:HG2	2.41	0.55
1:B:423:ASN:C	1:B:425:GLN:H	2.10	0.55
1:B:263:PRO:HD2	1:B:294:ILE:CD1	2.37	0.55
1:B:272:LYS:HD3	1:B:341:HIS:CD2	2.41	0.55
1:B:426:HIS:HE1	1:B:430:LEU:HD21	1.71	0.55
1:B:386:VAL:HG22	1:B:434:LEU:HD21	1.89	0.55
1:B:398:ARG:HH11	1:B:398:ARG:HG2	1.72	0.55
2:C:10:ASP:O	2:C:11:LYS:C	2.44	0.55
1:A:395:ILE:O	1:A:395:ILE:HG13	2.06	0.54
1:A:424:PRO:C	1:A:426:HIS:N	2.60	0.54
1:B:388:LEU:HD23	1:B:408:LEU:HD11	1.89	0.54
1:A:314:ILE:HG23	2:C:5:LEU:HD23	1.90	0.54
1:B:335:LYS:HE3	1:B:336:LYS:NZ	2.22	0.54
1:A:323:GLU:CB	1:A:437:LEU:HD13	2.38	0.54
1:B:319:GLY:O	1:B:392:ARG:HD3	2.08	0.54
1:B:316:LEU:HG	1:B:395:ILE:HD11	1.89	0.54
1:A:299:THR:HB	1:A:387:ILE:HG21	1.88	0.54
1:A:355:SER:HB3	1:A:357:GLU:HG2	1.88	0.54
1:A:402:GLU:O	1:A:405:GLN:N	2.41	0.54
1:A:323:GLU:CD	1:A:392:ARG:NH2	2.62	0.54
1:A:323:GLU:CD	1:A:392:ARG:HH22	2.11	0.53
1:A:354:ILE:HD13	1:A:355:SER:N	2.23	0.53
1:B:310:HIS:HA	1:B:313:GLN:HE21	1.73	0.53
1:A:447:MET:SD	1:A:447:MET:C	2.86	0.53
1:B:270:ILE:O	1:B:270:ILE:HG22	2.07	0.53
1:B:322:VAL:HG12	1:B:466:TRP:NE1	2.24	0.53
1:B:372:LEU:O	1:B:373:LYS:C	2.47	0.53
1:B:374:MET:CE	1:B:430:LEU:HD22	2.37	0.53
2:E:6:ARG:O	2:E:6:ARG:HD3	2.09	0.53
2:D:7:TYR:O	2:D:11:LYS:HB2	2.08	0.53
1:A:299:THR:HG21	1:A:317:LEU:HD21	1.90	0.53
1:A:306:GLN:HE21	1:A:306:GLN:CA	2.22	0.53
1:A:287:MET:O	1:A:290:SER:N	2.43	0.52
1:A:430:LEU:C	1:A:432:GLY:N	2.62	0.52
1:B:281:PHE:O	1:B:285:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:HG2	1:A:394:TYR:CD1	2.44	0.52
1:B:350:ARG:NH1	5:B:15:HOH:O	2.42	0.52
1:A:377:GLU:O	1:A:381:LEU:HD12	2.09	0.52
1:B:322:VAL:CG2	1:B:323:GLU:N	2.73	0.52
1:B:372:LEU:O	1:B:374:MET:N	2.42	0.52
1:A:326:PHE:HD2	1:A:366:TYR:HH	1.57	0.52
1:B:242:LEU:HG	1:B:246:GLN:CB	2.40	0.52
1:A:413:GLN:O	1:A:416:CYS:HB2	2.09	0.52
1:B:335:LYS:C	1:B:337:LEU:N	2.63	0.52
1:A:335:LYS:HZ3	1:A:373:LYS:HG2	1.74	0.52
1:A:417:LYS:O	1:A:421:PRO:HB3	2.10	0.52
1:A:310:HIS:CE1	2:C:9:LEU:HD23	2.44	0.52
1:B:447:MET:O	1:B:447:MET:CE	2.58	0.52
2:E:6:ARG:HG3	2:E:6:ARG:NH1	2.25	0.52
1:B:423:ASN:O	1:B:425:GLN:N	2.43	0.51
1:A:282:LEU:CA	1:A:285:THR:HG22	2.39	0.51
1:A:454:ASN:N	1:A:454:ASN:HD22	2.08	0.51
1:A:360:THR:N	1:A:361:PRO:HD2	2.26	0.51
1:A:430:LEU:O	1:A:432:GLY:N	2.43	0.51
1:B:362:MET:O	1:B:365:PHE:HB3	2.11	0.51
1:A:282:LEU:HA	1:A:285:THR:CG2	2.41	0.51
1:A:422:GLU:CD	1:A:422:GLU:H	2.14	0.51
1:A:314:ILE:O	1:A:317:LEU:N	2.44	0.51
1:B:423:ASN:HD21	1:B:425:GLN:HB2	1.75	0.51
1:A:254:MET:SD	1:A:377:GLU:HA	2.51	0.51
1:A:337:LEU:C	1:A:339:ALA:H	2.14	0.51
1:A:299:THR:HA	1:A:302:LEU:HD22	1.92	0.51
1:B:311:GLU:N	1:B:311:GLU:CD	2.64	0.50
1:A:424:PRO:HG2	1:A:425:GLN:N	2.21	0.50
1:B:359:ILE:C	1:B:361:PRO:HD2	2.31	0.50
1:B:299:THR:HG22	1:B:387:ILE:HG21	1.93	0.50
1:A:283:ILE:CD1	1:A:348:ARG:HH21	2.24	0.50
1:B:264:GLN:HG3	2:E:5:LEU:CD1	2.42	0.50
1:B:447:MET:HE3	1:B:451:TRP:HB2	1.94	0.50
1:B:280:ASN:OD1	1:B:348:ARG:HD3	2.11	0.50
1:B:302:LEU:O	1:B:303:PRO:C	2.48	0.50
1:B:452:ARG:HH21	1:B:453:VAL:HA	1.77	0.50
1:B:260:GLN:O	1:B:261:ARG:NH1	2.44	0.50
1:B:322:VAL:HG12	1:B:466:TRP:HE1	1.77	0.50
1:A:341:HIS:HA	1:A:344:LEU:HG	1.93	0.49
1:A:291:HIS:NE2	1:A:328:ARG:HG3	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:PRO:O	1:B:339:ALA:HB3	2.12	0.49
2:D:7:TYR:CZ	2:D:11:LYS:HG3	2.48	0.49
1:A:252:TYR:O	1:A:255:ASP:HB3	2.12	0.49
2:D:5:LEU:HD13	2:D:5:LEU:O	2.12	0.49
1:B:265:GLU:HA	1:B:265:GLU:OE1	2.12	0.49
1:B:269:LYS:O	1:B:271:LEU:N	2.46	0.49
1:A:290:SER:O	1:A:293:GLN:N	2.41	0.49
1:B:280:ASN:O	1:B:284:LEU:HG	2.13	0.49
1:B:381:LEU:O	1:B:385:ILE:HG13	2.13	0.49
1:B:268:ASN:N	1:B:268:ASN:HD22	2.11	0.48
1:B:299:THR:O	1:B:302:LEU:HB2	2.13	0.48
1:B:336:LYS:C	1:B:338:PRO:HD2	2.34	0.48
1:A:423:ASN:CB	1:A:424:PRO:CA	2.91	0.48
1:B:453:VAL:HG12	1:B:456:HIS:HB2	1.95	0.48
1:A:354:ILE:HG23	1:A:354:ILE:O	2.12	0.48
1:A:391:ASP:O	1:A:438:ARG:NH2	2.46	0.48
1:A:308:LEU:HD11	1:A:404:LEU:HD22	1.95	0.48
1:A:406:GLU:HB2	1:A:407:PRO:HD3	1.96	0.48
1:A:432:GLY:O	1:A:435:THR:N	2.47	0.48
1:B:333:PHE:C	1:B:335:LYS:H	2.16	0.48
1:B:377:GLU:OE1	1:B:419:TYR:HE1	1.96	0.48
1:B:438:ARG:HA	1:B:441:ASN:HD22	1.78	0.48
1:B:450:SER:O	1:B:452:ARG:HG3	2.14	0.47
1:A:467:ASP:C	1:A:468:VAL:HG22	2.35	0.47
1:A:330:ALA:HB1	1:A:369:VAL:HG21	1.96	0.47
1:B:288:ALA:O	1:B:289:THR:C	2.52	0.47
1:A:390:PRO:HD3	1:A:405:GLN:OE1	2.15	0.47
1:B:263:PRO:O	1:B:264:GLN:CB	2.58	0.47
1:B:328:ARG:HE	4:B:1002:IU5:C24	2.27	0.47
2:C:1:GLU:OE1	2:C:1:GLU:HA	2.15	0.47
1:A:244:VAL:HG23	1:A:245:ASP:N	2.29	0.47
1:A:241:GLU:CD	1:A:241:GLU:N	2.59	0.47
1:B:438:ARG:O	1:B:441:ASN:HB2	2.15	0.47
1:B:337:LEU:O	1:B:338:PRO:C	2.53	0.47
1:A:283:ILE:HG22	1:A:284:LEU:N	2.28	0.47
1:A:389:SER:CB	1:A:392:ARG:HH11	2.27	0.47
1:A:437:LEU:HA	1:A:440:PHE:HB2	1.96	0.47
1:B:406:GLU:N	1:B:407:PRO:HD2	2.30	0.47
1:A:385:ILE:HD11	1:A:434:LEU:HD22	1.97	0.46
1:B:438:ARG:HH11	1:B:438:ARG:HG2	1.80	0.46
1:A:323:GLU:O	1:A:326:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:O	1:B:253:ILE:HG13	2.16	0.46
1:B:374:MET:CE	1:B:382:LEU:HD11	2.46	0.46
1:B:337:LEU:HB3	1:B:338:PRO:HD3	1.98	0.46
1:A:256:SER:O	1:A:301:ARG:NH2	2.48	0.46
1:B:407:PRO:O	1:B:410:ASP:HB3	2.16	0.46
1:A:437:LEU:HA	1:A:440:PHE:HD2	1.80	0.46
1:B:360:THR:N	1:B:361:PRO:CD	2.79	0.46
1:B:272:LYS:HZ3	1:B:272:LYS:HB2	1.81	0.46
1:B:392:ARG:NH1	1:B:438:ARG:NH2	2.64	0.46
1:B:331:GLU:O	1:B:333:PHE:O	2.34	0.45
1:B:350:ARG:CZ	5:B:15:HOH:O	2.65	0.45
1:B:264:GLN:NE2	2:E:2:ASN:HB2	2.31	0.45
1:B:452:ARG:NE	1:B:453:VAL:N	2.63	0.45
1:B:465:ILE:HG23	2:D:5:LEU:CD2	2.46	0.45
1:A:422:GLU:N	1:A:422:GLU:OE2	2.50	0.45
1:A:442:HIS:HB2	1:B:402:GLU:OE1	2.15	0.45
1:B:267:THR:O	1:B:268:ASN:C	2.55	0.45
1:A:391:ASP:HA	1:A:398:ARG:NH1	2.31	0.45
1:A:430:LEU:O	1:A:431:LEU:C	2.51	0.45
1:B:318:LYS:O	1:B:320:SER:N	2.50	0.45
1:B:339:ALA:O	1:B:341:HIS:CD2	2.70	0.45
1:A:278:GLU:HB2	1:A:456:HIS:CD2	2.50	0.45
1:A:467:ASP:O	1:A:468:VAL:HG13	2.17	0.45
1:B:272:LYS:O	1:B:273:GLU:OE1	2.35	0.45
1:B:465:ILE:HD12	1:B:466:TRP:N	2.32	0.45
1:A:300:LYS:O	1:A:306:GLN:NE2	2.48	0.45
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.88	0.45
1:A:335:LYS:CE	1:A:373:LYS:HG2	2.47	0.45
1:B:374:MET:HE3	1:B:382:LEU:HD11	1.98	0.45
1:A:276:SER:HB2	1:A:279:GLU:HB2	1.97	0.44
1:B:278:GLU:OE1	1:B:278:GLU:C	2.55	0.44
1:B:363:PHE:O	1:B:367:LYS:HB2	2.17	0.44
1:B:268:ASN:ND2	1:B:268:ASN:N	2.65	0.44
1:B:446:GLU:O	1:B:448:LEU:N	2.50	0.44
1:A:275:PHE:HB3	1:A:276:SER:H	1.39	0.44
1:A:395:ILE:CD1	1:A:398:ARG:HG2	2.47	0.44
1:A:423:ASN:HD22	1:A:424:PRO:CA	2.27	0.44
1:B:318:LYS:HZ1	2:D:2:ASN:HD21	1.60	0.44
1:B:311:GLU:CD	1:B:311:GLU:H	2.21	0.44
1:B:411:VAL:HG12	1:B:415:LEU:HD22	1.99	0.44
1:A:355:SER:C	1:A:357:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASN:N	1:A:454:ASN:ND2	2.66	0.44
1:B:423:ASN:C	1:B:425:GLN:N	2.71	0.44
1:A:361:PRO:O	1:A:364:SER:HB3	2.18	0.44
1:B:284:LEU:HD11	1:B:349:ILE:HA	1.99	0.44
1:B:346:GLU:O	1:B:349:ILE:HB	2.18	0.44
1:B:388:LEU:O	1:B:405:GLN:OE1	2.35	0.44
1:A:424:PRO:O	1:A:426:HIS:N	2.50	0.44
1:B:271:LEU:O	1:B:344:LEU:HD21	2.18	0.44
1:B:390:PRO:HD3	1:B:405:GLN:OE1	2.18	0.44
1:A:327:LEU:O	1:A:330:ALA:HB3	2.18	0.44
1:B:262:MET:HG3	1:B:262:MET:O	2.18	0.44
1:B:332:ILE:HD11	4:B:1002:IU5:O4	2.18	0.44
1:B:393:GLN:O	1:B:394:TYR:CB	2.65	0.44
1:A:272:LYS:C	1:A:273:GLU:O	2.56	0.43
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.75	0.43
1:A:395:ILE:HD12	1:A:401:VAL:HG21	2.01	0.43
1:B:295:LEU:O	1:B:299:THR:HG23	2.18	0.43
1:A:359:ILE:O	1:A:363:PHE:HB2	2.19	0.43
1:A:424:PRO:CG	1:A:425:GLN:N	2.81	0.43
1:B:335:LYS:HE3	1:B:336:LYS:HZ3	1.83	0.43
1:A:346:GLU:O	1:A:350:ARG:HG2	2.17	0.43
1:A:275:PHE:O	1:A:276:SER:HB2	2.18	0.43
1:A:368:SER:O	1:A:371:GLU:HB2	2.18	0.43
1:A:451:TRP:C	1:A:452:ARG:HA	2.38	0.43
1:B:292:VAL:HG12	1:B:461:LEU:HD21	2.00	0.43
1:A:292:VAL:CG1	1:A:465:ILE:HD13	2.49	0.43
1:B:372:LEU:O	1:B:374:MET:HG2	2.19	0.43
1:B:254:MET:SD	1:B:377:GLU:HA	2.59	0.42
1:B:358:TYR:CE1	1:B:362:MET:HE2	2.54	0.42
1:A:350:ARG:NH1	1:A:359:ILE:HG13	2.34	0.42
1:A:354:ILE:HG12	1:A:447:MET:HE2	1.99	0.42
1:B:398:ARG:HG2	1:B:398:ARG:NH1	2.33	0.42
2:D:6:ARG:HB3	2:D:6:ARG:HH11	1.84	0.42
1:B:265:GLU:HB3	1:B:269:LYS:HE3	2.01	0.42
1:B:446:GLU:C	1:B:448:LEU:N	2.73	0.42
1:B:317:LEU:HG	2:D:5:LEU:HD11	2.00	0.42
1:A:335:LYS:HZ1	1:A:373:LYS:HG2	1.79	0.42
1:B:292:VAL:HG12	1:B:293:GLN:N	2.34	0.42
1:B:299:THR:C	1:B:301:ARG:H	2.23	0.42
1:A:453:VAL:O	1:A:454:ASN:HB2	2.20	0.42
1:A:299:THR:CG2	1:A:317:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:O	1:A:363:PHE:HD1	2.03	0.42
1:B:278:GLU:C	1:B:280:ASN:N	2.73	0.42
1:B:461:LEU:HD13	2:D:4:LEU:HD22	2.02	0.42
1:A:360:THR:H	1:A:361:PRO:HD2	1.85	0.41
1:B:293:GLN:HE22	2:E:5:LEU:HG	1.85	0.41
1:B:352:SER:O	1:B:354:ILE:N	2.51	0.41
1:B:243:THR:O	1:B:246:GLN:N	2.51	0.41
1:B:333:PHE:C	1:B:335:LYS:N	2.73	0.41
1:A:318:LYS:HE2	5:A:14:HOH:O	2.19	0.41
1:B:335:LYS:O	1:B:337:LEU:N	2.53	0.41
1:A:354:ILE:HG23	1:A:359:ILE:HG21	2.02	0.41
1:A:390:PRO:HG2	1:A:402:GLU:HG2	2.03	0.41
1:A:423:ASN:CB	1:A:424:PRO:O	2.60	0.41
1:B:321:ALA:O	1:B:324:ALA:N	2.53	0.41
1:A:266:ILE:HD13	1:A:286:GLU:HG2	2.01	0.41
1:A:326:PHE:HD2	1:A:366:TYR:OH	2.03	0.41
1:A:354:ILE:HD13	1:A:354:ILE:C	2.40	0.41
1:B:452:ARG:O	1:B:453:VAL:HG12	2.20	0.41
1:A:448:LEU:HD11	1:A:466:TRP:HB3	2.03	0.41
1:B:264:GLN:HG3	2:E:5:LEU:HD13	2.02	0.41
1:B:354:ILE:HG22	1:B:451:TRP:CD1	2.55	0.41
1:B:460:PRO:O	1:B:461:LEU:C	2.57	0.41
1:A:270:ILE:HG22	1:A:283:ILE:HG21	2.01	0.41
1:A:302:LEU:HD23	1:A:388:LEU:HD21	2.03	0.41
1:A:347:GLU:O	1:A:350:ARG:O	2.39	0.41
1:B:459:THR:O	1:B:460:PRO:C	2.59	0.41
1:A:354:ILE:HD11	1:A:358:TYR:HB3	2.01	0.41
1:A:404:LEU:N	1:A:404:LEU:HD12	2.36	0.41
1:B:262:MET:N	1:B:263:PRO:CD	2.84	0.41
1:A:366:TYR:O	1:A:369:VAL:HG22	2.21	0.41
1:B:392:ARG:HH11	1:B:438:ARG:NH2	2.19	0.41
1:B:270:ILE:O	1:B:270:ILE:CG2	2.69	0.40
1:B:415:LEU:HD12	1:B:415:LEU:HA	1.87	0.40
1:B:467:ASP:O	1:B:468:VAL:C	2.59	0.40
1:A:403:LYS:O	1:A:407:PRO:CD	2.70	0.40
1:A:390:PRO:HA	1:A:395:ILE:CD1	2.51	0.40
1:B:260:GLN:HB2	1:B:294:ILE:HG23	2.02	0.40
1:B:320:SER:HA	1:B:392:ARG:NH2	2.36	0.40
1:A:316:LEU:HD22	1:A:387:ILE:O	2.22	0.40
1:A:322:VAL:HG21	1:A:441:ASN:OD1	2.21	0.40
1:A:349:ILE:CG2	3:A:1001:CHC:H253	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:MET:HB2	1:B:379:TYR:HE1	1.72	0.40
2:C:6:ARG:HE	2:C:6:ARG:HB2	1.56	0.40
1:B:309:ASP:O	1:B:313:GLN:HG3	2.22	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	225/229 (98%)	165 (73%)	45 (20%)	15 (7%)	1	3
1	B	227/229 (99%)	168 (74%)	39 (17%)	20 (9%)	1	2
2	C	10/12 (83%)	7 (70%)	1 (10%)	2 (20%)	0	0
2	D	10/12 (83%)	5 (50%)	4 (40%)	1 (10%)	0	1
2	E	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
All	All	482/494 (98%)	354 (73%)	90 (19%)	38 (8%)	1	2

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	GLU
1	A	242	LEU
1	A	275	PHE
1	A	336	LYS
1	A	423	ASN
1	A	424	PRO
1	B	303	PRO
1	B	305	PHE
1	B	321	ALA
1	B	337	LEU
1	B	373	LYS

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Mol	Chain	Res	Type
1	B	455	ASP
2	D	11	LYS
1	A	333	PHE
1	A	342	ALA
1	A	393	GLN
1	A	455	ASP
1	B	264	GLN
1	B	339	ALA
1	B	453	VAL
1	B	467	ASP
2	C	2	ASN
2	C	11	LYS
1	A	260	GLN
1	B	319	GLY
1	B	447	MET
1	A	454	ASN
1	B	338	PRO
1	A	335	LYS
1	A	356	ASP
1	B	300	LYS
1	B	350	ARG
1	B	424	PRO
1	B	454	ASN
1	B	353	GLY
1	B	332	ILE
1	A	338	PRO
1	B	340	GLY

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	209/210 (100%)	191 (91%)	18 (9%)	10 30
1	B	209/210 (100%)	185 (88%)	24 (12%)	5 17
2	C	10/11 (91%)	10 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	11/11 (100%)	9 (82%)	2 (18%)	1 5
2	E	10/11 (91%)	8 (80%)	2 (20%)	1 4
All	All	449/453 (99%)	403 (90%)	46 (10%)	7 22

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	LEU
1	A	299	THR
1	A	302	LEU
1	A	306	GLN
1	A	328	ARG
1	A	341	HIS
1	A	354	ILE
1	A	356	ASP
1	A	359	ILE
1	A	371	GLU
1	A	376	GLN
1	A	385	ILE
1	A	392	ARG
1	A	406	GLU
1	A	409	LEU
1	A	423	ASN
1	A	433	ARG
1	A	468	VAL
1	B	273	GLU
1	B	275	PHE
1	B	278	GLU
1	B	279	GLU
1	B	302	LEU
1	B	303	PRO
1	B	317	LEU
1	B	327	LEU
1	B	337	LEU
1	B	338	PRO
1	B	356	ASP
1	B	377	GLU
1	B	388	LEU
1	B	405	GLN
1	B	415	LEU
1	B	422	GLU

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Mol	Chain	Res	Type
1	B	423	ASN
1	B	433	ARG
1	B	438	ARG
1	B	447	MET
1	B	449	MET
1	B	452	ARG
1	B	453	VAL
1	B	467	ASP
2	D	1	GLU
2	D	5	LEU
2	E	5	LEU
2	E	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	293	GLN
1	A	306	GLN
1	A	310	HIS
1	A	334	ASN
1	A	376	GLN
1	A	423	ASN
1	A	425	GLN
1	A	444	HIS
1	A	454	ASN
1	B	264	GLN
1	B	268	ASN
1	B	313	GLN
1	B	334	ASN
1	B	341	HIS
1	B	376	GLN
1	B	405	GLN
1	B	413	GLN
1	B	420	GLN
1	B	423	ASN
1	B	426	HIS
1	B	441	ASN
1	B	456	HIS
2	D	2	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)

2 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	$\#\|Z\| > 2$
4	IU5	B	1002	-	30,30,31	2.57	15 (50%)	47,47,49	1.52	9 (19%)
3	CHC	A	1001	-	33,33,33	3.67	19 (57%)	52,52,52	1.77	11 (21%)

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	CHC	A	1001	-	-	2/11/76/76	0/4/4/4
4	IU5	B	1002	-	1/1/10/11	2/9/68/70	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	CHC	C10-C9	7.47	1.69	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	CHC	C4-C3	7.24	1.64	1.52
3	A	1001	CHC	C18-C13	6.35	1.64	1.54
3	A	1001	CHC	C4-C5	6.08	1.63	1.53
3	A	1001	CHC	C8-C9	6.07	1.65	1.53
3	A	1001	CHC	C10-C5	5.77	1.66	1.56
3	A	1001	CHC	C6-C7	5.06	1.58	1.53
4	B	1002	IU5	C10-C5	4.90	1.63	1.55
4	B	1002	IU5	C10-C9	4.87	1.64	1.56
4	B	1002	IU5	C18-C13	4.84	1.62	1.54
3	A	1001	CHC	C20-C17	4.38	1.61	1.54
4	B	1002	IU5	C4-C5	3.93	1.62	1.53
3	A	1001	CHC	C21-C20	3.70	1.62	1.53
3	A	1001	CHC	C13-C17	3.62	1.61	1.55
4	B	1002	IU5	C8-C14	3.62	1.60	1.53
3	A	1001	CHC	C6-C5	3.60	1.60	1.53
3	A	1001	CHC	C2-C3	3.59	1.60	1.51
3	A	1001	CHC	C1-C10	3.58	1.60	1.54
4	B	1002	IU5	C21-C20	3.51	1.62	1.53
4	B	1002	IU5	C8-C7	3.46	1.59	1.53
3	A	1001	CHC	C8-C7	3.37	1.58	1.53
3	A	1001	CHC	C8-C14	3.12	1.59	1.53
4	B	1002	IU5	O1A-C7	3.10	1.49	1.43
3	A	1001	CHC	C16-C17	3.08	1.60	1.54
3	A	1001	CHC	C12-C11	3.05	1.59	1.53
4	B	1002	IU5	C1-C10	3.04	1.59	1.54
3	A	1001	CHC	C15-C14	2.92	1.60	1.54
4	B	1002	IU5	C20-C17	2.90	1.59	1.54
3	A	1001	CHC	C12-C13	2.72	1.58	1.54
4	B	1002	IU5	C6-C5	2.72	1.58	1.53
4	B	1002	IU5	C16-C17	2.52	1.59	1.54
4	B	1002	IU5	C8-C9	2.34	1.58	1.53
4	B	1002	IU5	C13-C17	2.23	1.59	1.55
4	B	1002	IU5	C11-C9	2.11	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	CHC	C26-C6-C7	-5.74	104.95	112.09
4	B	1002	IU5	C19-C10-C1	-5.27	99.93	108.31
3	A	1001	CHC	C19-C10-C1	-4.17	101.68	108.31
3	A	1001	CHC	C10-C5-C6	-3.74	108.63	112.43
3	A	1001	CHC	C16-C15-C14	-3.30	98.69	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	CHC	C4-C5-C10	-2.75	109.16	112.25
4	B	1002	IU5	C16-C15-C14	-2.70	99.85	105.14
4	B	1002	IU5	C19-C10-C5	2.47	114.56	110.44
4	B	1002	IU5	C4-C5-C10	-2.44	108.22	112.31
3	A	1001	CHC	C10-C9-C8	-2.44	109.12	111.84
3	A	1001	CHC	C26-C6-C5	-2.37	109.88	113.62
4	B	1002	IU5	C15-C14-C13	-2.29	101.15	103.84
4	B	1002	IU5	C17-C13-C14	-2.26	97.51	100.10
3	A	1001	CHC	C4-C5-C6	2.22	115.87	113.18
3	A	1001	CHC	C13-C17-C20	-2.22	116.07	119.50
4	B	1002	IU5	C13-C17-C20	-2.22	116.07	119.50
3	A	1001	CHC	C21-C20-C17	-2.20	109.58	112.88
3	A	1001	CHC	OT2-C24-C23	-2.16	116.25	123.09
4	B	1002	IU5	C5-C6-C7	-2.14	111.85	114.40
4	B	1002	IU5	C12-C13-C17	2.06	119.64	116.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1002	IU5	C7

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1002	IU5	C22-C23-C24-O4A
4	B	1002	IU5	C22-C23-C24-O4
3	A	1001	CHC	C22-C23-C24-OT2
3	A	1001	CHC	C22-C23-C24-OT1

There are no ring outliers.

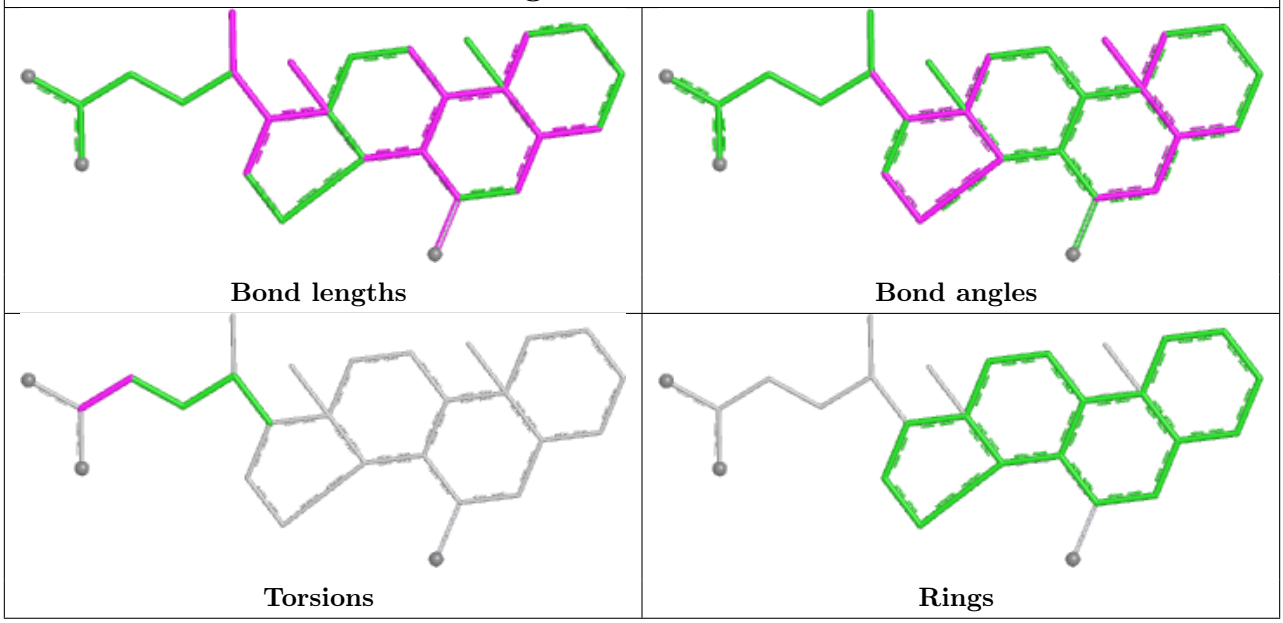
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	IU5	4	0
3	A	1001	CHC	3	0

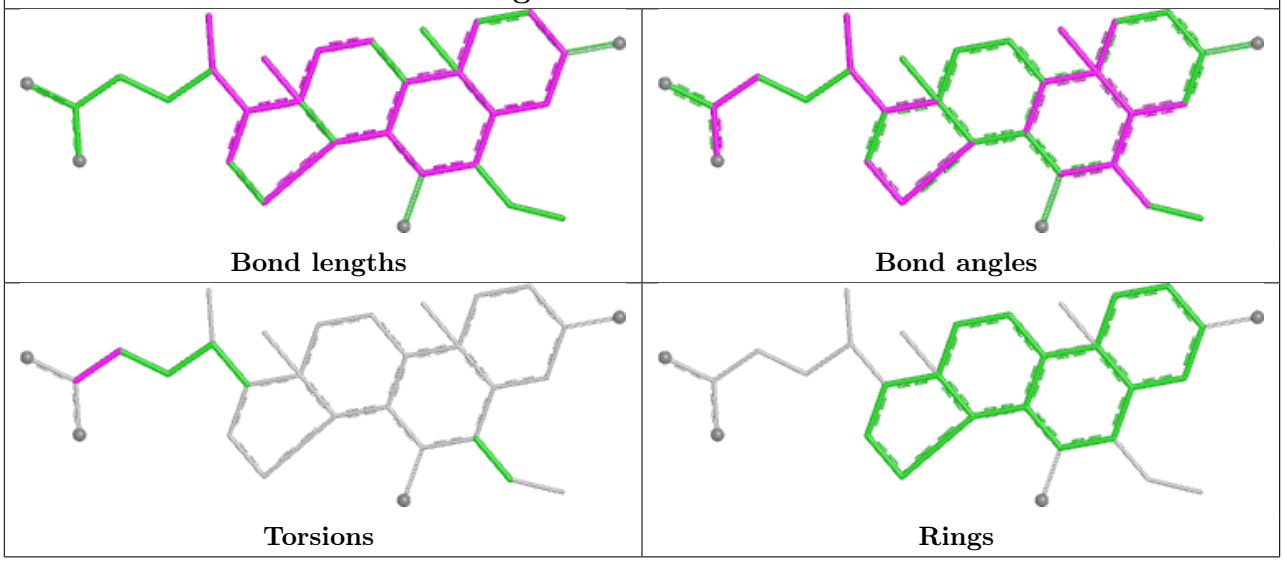
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 IU5 B 1002



Ligand CHC A 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	451:TRP	C	452:ARG	N	3.72

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	229/229 (100%)	0.35	23 (10%) 7 5	30, 78, 157, 191	9 (3%)
1	B	229/229 (100%)	0.10	13 (5%) 23 19	33, 69, 139, 183	1 (0%)
2	C	12/12 (100%)	0.50	1 (8%) 11 8	56, 68, 104, 187	0
2	D	12/12 (100%)	0.20	0 100 100	46, 70, 86, 105	0
2	E	12/12 (100%)	0.24	1 (8%) 11 8	62, 92, 124, 177	0
All	All	494/494 (100%)	0.23	38 (7%) 13 10	30, 73, 152, 191	10 (2%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	PHE	5.0
1	A	341	HIS	4.8
1	A	270	ILE	4.3
1	A	349	ILE	3.7
1	A	272	LYS	3.7
1	A	371	GLU	3.5
2	C	12	ASP	3.2
1	B	453	VAL	3.2
1	A	335	LYS	3.1
1	B	261	ARG	3.1
1	B	456	HIS	3.1
1	A	452	ARG	3.0
1	A	240	THR	2.9
1	A	339	ALA	2.9
1	B	336	LYS	2.8
1	B	468	VAL	2.8
1	A	277	ALA	2.8
1	A	278	GLU	2.7
1	A	348	ARG	2.7
1	A	351	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	337	LEU	2.5
1	B	455	ASP	2.5
1	A	354	ILE	2.4
1	A	284	LEU	2.4
1	A	260	GLN	2.4
1	A	372	LEU	2.4
1	B	341	HIS	2.3
1	A	281	PHE	2.3
1	B	454	ASN	2.3
1	A	273	GLU	2.2
1	B	264	GLN	2.1
1	B	452	ARG	2.1
1	A	338	PRO	2.1
1	B	262	MET	2.1
1	A	359	ILE	2.1
1	A	255	ASP	2.0
1	B	275	PHE	2.0
2	E	12	ASP	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.

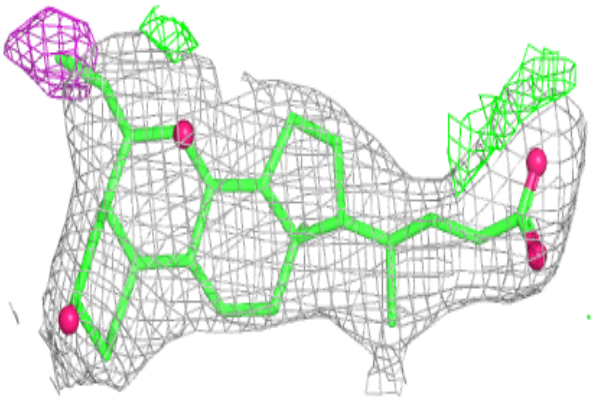
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CHC	A	1001	30/30	0.84	0.26	23,60,63,65	0
4	IU5	B	1002	27/28	0.93	0.25	40,43,49,52	0

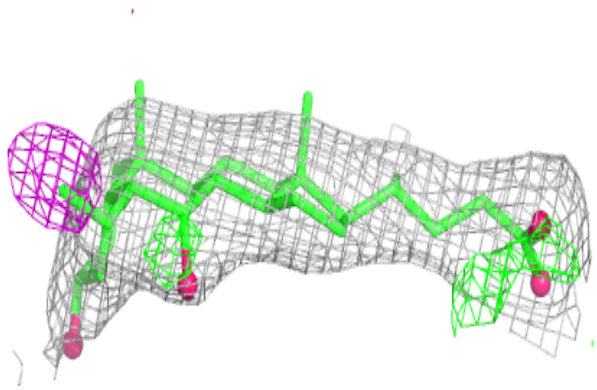
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

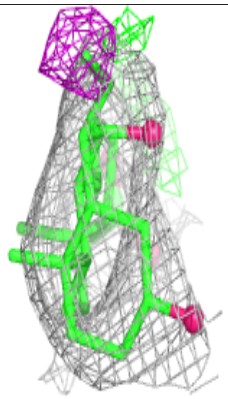
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CHC A 1001:

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

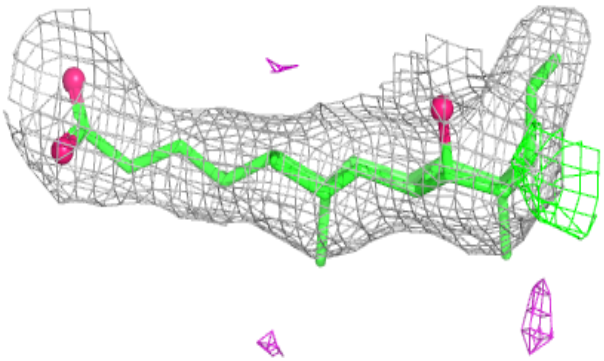


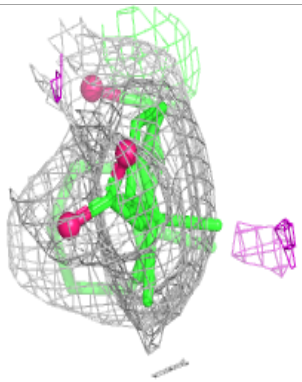




Electron density around IU5 B 1002:

$2mF_o$-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.