



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 1OT7 / pdb_00001ot7
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

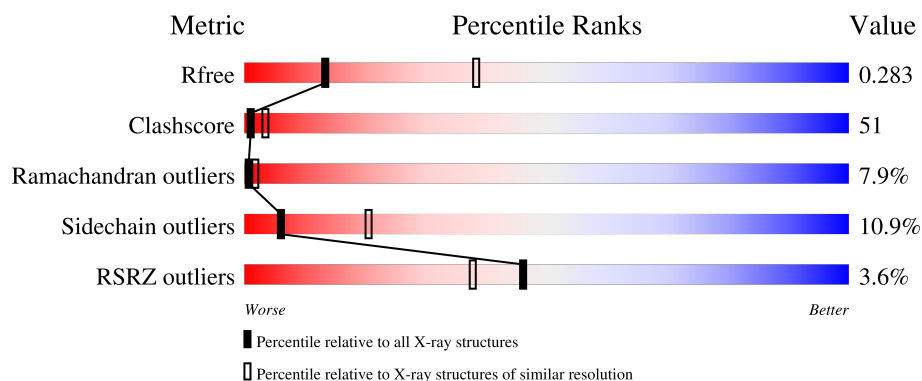
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	4% 31% 54% 14%
1	B	229	4% 33% 51% 13%
2	C	12	42% 33% 25%
2	D	12	33% 50% 17%
2	E	12	58% 33% 8%

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.

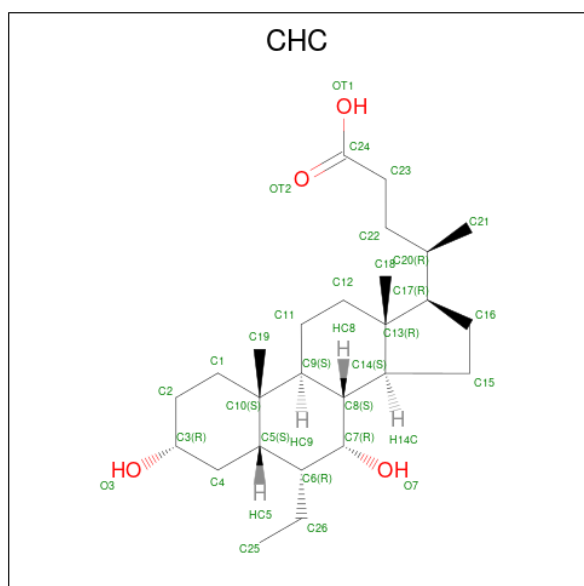
- Molecule 1 is a protein called Bile Acid Receptor.

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

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

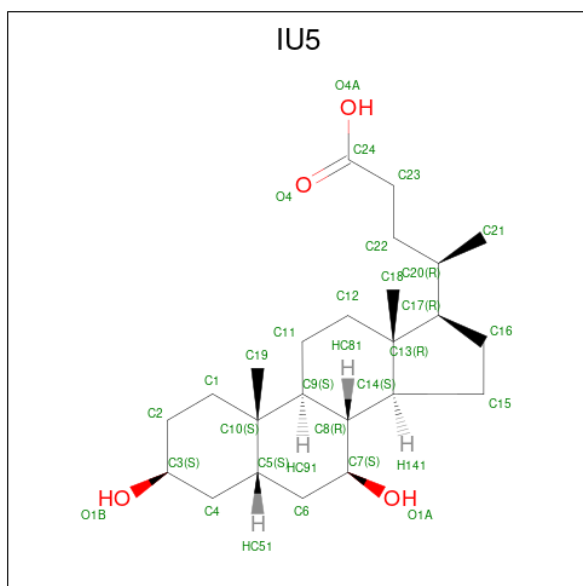
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			100	64	17	19			
2	D	12	Total	C	N	O	0	0	0
			103	65	17	21			
2	E	12	Total	C	N	O	0	0	0
			100	64	17	19			

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



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

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



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

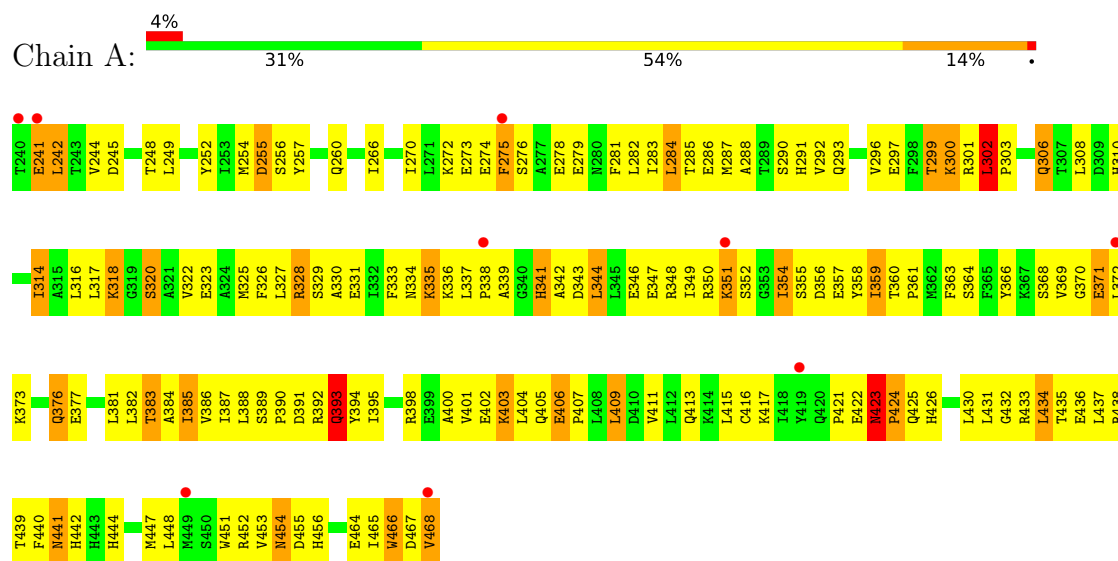
- Molecule 5 is water.

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

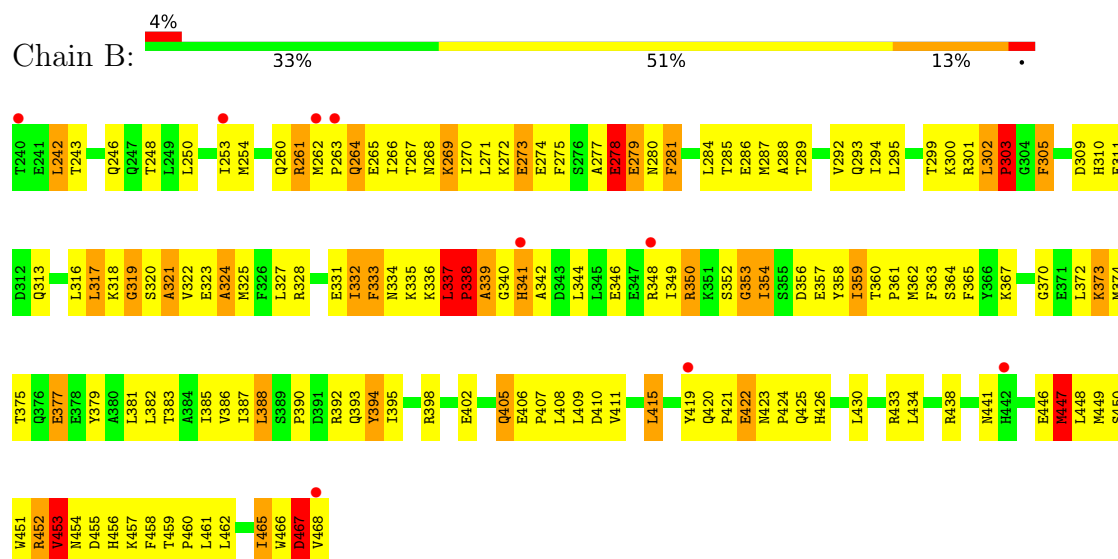
3 Residue-property plots

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.

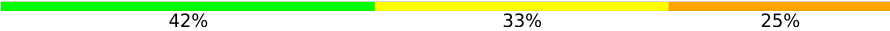
• Molecule 1: Bile Acid Receptor

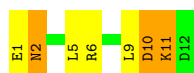


• Molecule 1: Bile Acid Receptor

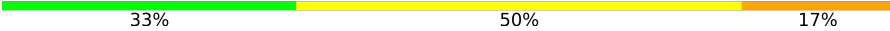


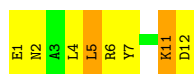
• Molecule 2: dodecamer peptide fragment of RPGR-interacting protein 1

Chain C:  42% 33% 25%



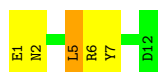
- Molecule 2: dodecamer peptide fragment of RPGR-interacting protein 1

Chain D:  33% 50% 17%



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

Chain E:  58% 33% 8%



4 Data and refinement statistics

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 19.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	75.4 (19.96-2.90) 98.4 (19.96-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.279 0.237 , 0.283	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)	0.25 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IU5, CHC

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	0.52	1/1913 (0.1%)	1.07	11/2581 (0.4%)
1	B	0.55	0/1914	1.11	14/2584 (0.5%)
2	C	0.50	0/100	0.99	1/132 (0.8%)
2	D	0.44	0/103	0.78	0/136
2	E	0.42	0/100	0.95	1/132 (0.8%)
All	All	0.53	1/4130 (0.0%)	1.07	27/5565 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	THR	CA-CB	5.50	1.62	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	ALA	N-CA-C	-8.99	101.05	111.03
1	B	341	HIS	N-CA-C	8.05	123.20	112.25
1	B	359	ILE	N-CA-C	7.83	117.78	110.42
1	B	281	PHE	N-CA-C	-7.72	102.46	111.03
1	B	278	GLU	N-CA-C	-7.66	103.91	113.18
1	A	255	ASP	N-CA-C	-7.52	101.54	111.24
1	A	274	GLU	N-CA-C	7.20	120.68	109.52
1	B	364	SER	N-CA-C	-7.14	103.57	111.36
1	A	343	ASP	N-CA-C	-6.93	103.78	111.82
1	A	441	ASN	N-CA-C	-6.61	104.48	112.54
1	A	393	GLN	N-CA-C	6.59	124.83	110.80
1	B	333	PHE	N-CA-C	-6.57	101.86	110.53
1	A	318	LYS	N-CA-C	-6.28	103.58	111.11
1	A	302	LEU	N-CA-C	-6.21	99.95	109.64
1	B	357	GLU	N-CA-C	-6.06	104.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	10	ASP	N-CA-C	-5.96	102.66	110.53
1	B	356	ASP	N-CA-C	-5.93	106.01	113.18
1	A	320	SER	N-CA-C	5.70	120.37	112.90
1	B	305	PHE	N-CA-C	5.69	122.92	110.80
1	A	314	ILE	N-CA-C	-5.67	104.80	110.30
1	A	466	TRP	N-CA-C	-5.54	105.83	112.59
1	B	324	ALA	N-CA-C	-5.51	104.96	110.97
2	E	7	TYR	N-CA-C	-5.50	106.24	113.12
1	A	383	THR	CB-CA-C	-5.22	102.68	110.88
1	B	248	THR	N-CA-C	-5.11	105.60	111.07
1	B	467	ASP	N-CA-C	5.11	121.69	110.80
1	B	394	TYR	N-CA-CB	-5.07	109.03	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	185	0
1	B	1876	0	1876	224	0
2	C	100	0	104	6	0
2	D	103	0	106	11	0
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	11	0
5	D	3	0	0	0	0
All	All	4140	0	4145	420	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 51.

All (420) 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:374:MET:HE1	1:B:382:LEU:HD11	1.49	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:A:241:GLU:H	1:A:241:GLU:CD	1.83	0.86
1:B:374:MET:HB2	1:B:379:TYR:CE1	2.10	0.86
1:B:325:MET:HE1	4:B:1002:IU5:HC21	1.58	0.85
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:374:MET:HE3	1:B:430:LEU:HD22	1.61	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: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
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:A:424:PRO:C	1:A:426:HIS:H	1.90	0.78
1:B:447:MET:HE2	1:B:447:MET:O	1.84	0.77
1:A:323:GLU:HB3	1:A:437:LEU:HD13	1.67	0.77
1:A:354:ILE:HG12	1:A:447:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:254:MET:HE1	1:A:376:GLN:HB3	1.68	0.74
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: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:447:MET:HE1	1:B:451:TRP:CE3	2.24	0.72
1:A:423:ASN:HB2	1:A:424:PRO:C	2.14	0.71
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:B:374:MET:HE1	1:B:382:LEU:CD1	2.20	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: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:A:451:TRP:C	1:A:452:ARG:HD3	2.17	0.68
1:A:354:ILE:HG12	1:A:447:MET:CE	2.22	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HD11	1:A:398:ARG:HG2	1.77	0.66
1:A:349:ILE:HG21	3:A:1001:CHC:H253	1.77	0.65
1:A:464:GLU:CD	2:C:2:ASN:HA	2.21	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:422:GLU:CD	1:B:422:GLU:H	2.04	0.65
1:B:321:ALA:O	1:B:324:ALA:HB3	1.96	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:B:375:THR:OG1	1:B:377:GLU:HG2	1.98	0.64
1:B:269:LYS:C	1:B:271:LEU:H	2.06	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:A:335:LYS:HZ1	1:A:373:LYS:HG2	1.64	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:318:LYS:HZ2	2:D:2:ASN:HD21	1.48	0.61
1:B:336:LYS:O	1:B:337:LEU:HB2	2.00	0.61
1:B:447:MET:HE2	1:B:447:MET:C	2.25	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:292:VAL:O	1:B:295:LEU:N	2.33	0.60
1:A:257:TYR:OH	1:A:331:GLU:OE2	2.20	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:269:LYS:C	1:B:271:LEU:N	2.57	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:ASN:C	1:B:425:GLN:H	2.10	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
2:C:10:ASP:O	2:C:11:LYS:C	2.44	0.59
1:B:266:ILE:O	1:B:270:ILE:HG13	2.03	0.59
1:A:241:GLU:CD	1:A:241:GLU:N	2.59	0.59
1:A:325:MET:O	1:A:329:SER:OG	2.14	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:323:GLU:CD	1:A:392:ARG:NH2	2.62	0.58
1:A:296:VAL:HG12	1:A:296:VAL:O	2.03	0.58
1:A:323:GLU:CD	1:A:392:ARG:HH22	2.11	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:447:MET:SD	1:A:447:MET:C	2.86	0.58
1:B:372:LEU:O	1:B:373:LYS:C	2.47	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: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: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:325:MET:CE	4:B:1002:IU5:HC21	2.32	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:A:422:GLU:CD	1:A:422:GLU:H	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:HG21	1:A:465:ILE:CD1	2.37	0.55
1:A:337:LEU:C	1:A:339:ALA:H	2.14	0.55
1:B:336:LYS:O	1:B:337:LEU:CB	2.55	0.55
1:B:311:GLU:N	1:B:311:GLU:CD	2.64	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:B:359:ILE:C	1:B:361:PRO:HD2	2.31	0.55
1:A:358:TYR:CE1	1:A:447:MET:HG2	2.41	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:302:LEU:O	1:B:303:PRO:C	2.48	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
1:A:395:ILE:O	1:A:395:ILE:HG13	2.06	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:333:PHE:C	1:B:335:LYS:H	2.16	0.54
1:A:430:LEU:C	1:A:432:GLY:N	2.62	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: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:B:335:LYS:C	1:B:337:LEU:N	2.63	0.53
1:A:424:PRO:C	1:A:426:HIS:N	2.60	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
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:B:281:PHE:O	1:B:285:THR:HG23	2.10	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:VAL:CG2	1:B:323:GLU:N	2.73	0.52
1:B:336:LYS:C	1:B:338:PRO:HD2	2.34	0.52
1:B:372:LEU:O	1:B:374:MET:N	2.42	0.52
1:B:242:LEU:HG	1:B:246:GLN:CB	2.40	0.52
1:B:288:ALA:O	1:B:289:THR:C	2.52	0.52
1:A:413:GLN:O	1:A:416:CYS:HB2	2.09	0.52
1:A:417:LYS:O	1:A:421:PRO:HB3	2.10	0.52
1:A:467:ASP:C	1:A:468:VAL:HG22	2.35	0.52
1:A:310:HIS:CE1	2:C:9:LEU:HD23	2.44	0.52
2:E:6:ARG:HG3	2:E:6:ARG:NH1	2.25	0.52
1:B:337:LEU:O	1:B:338:PRO:C	2.53	0.51
1:B:374:MET:CE	1:B:430:LEU:HD22	2.37	0.51
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: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:299:THR:HA	1:A:302:LEU:HD22	1.92	0.51
1:A:424:PRO:HG2	1:A:425:GLN:N	2.21	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:280:ASN:OD1	1:B:348:ARG:HD3	2.11	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:267:THR:O	1:B:268:ASN:C	2.55	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
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
1:A:430:LEU:O	1:A:431:LEU:C	2.51	0.49
2:D:5:LEU:HD13	2:D:5:LEU:O	2.12	0.49
1:B:278:GLU:OE1	1:B:278:GLU:C	2.55	0.49
1:B:265:GLU:HA	1:B:265:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LYS:O	1:B:271:LEU:N	2.46	0.49
1:B:447:MET:O	1:B:447:MET:CE	2.58	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:311:GLU:CD	1:B:311:GLU:H	2.21	0.49
1:B:381:LEU:O	1:B:385:ILE:HG13	2.13	0.49
1:B:423:ASN:C	1:B:425:GLN:N	2.71	0.49
1:A:355:SER:C	1:A:357:GLU:H	2.20	0.48
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: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:272:LYS:C	1:A:273:GLU:O	2.56	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:A:451:TRP:C	1:A:452:ARG:HA	2.38	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:272:LYS:HZ3	1:B:272:LYS:HB2	1.79	0.47
1:B:450:SER:O	1:B:452:ARG:HG3	2.14	0.47
1:A:330:ALA:HB1	1:A:369:VAL:HG21	1.96	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:B:438:ARG:O	1:B:441:ASN:HB2	2.15	0.47
1:B:446:GLU:C	1:B:448:LEU:N	2.73	0.47
1:A:351:LYS:HZ3	1:A:351:LYS:N	2.13	0.47
1:B:299:THR:C	1:B:301:ARG:H	2.23	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
1:B:250:LEU:O	1:B:253:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:PHE:C	1:B:335:LYS:N	2.73	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:354:ILE:HD13	1:A:354:ILE:C	2.40	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:374:MET:HE3	1:B:430:LEU:CD2	2.39	0.46
1:B:460:PRO:O	1:B:461:LEU:C	2.57	0.46
1:B:392:ARG:NH1	1:B:438:ARG:NH2	2.64	0.46
1:B:459:THR:O	1:B:460:PRO:C	2.59	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:A:335:LYS:HZ1	1:A:373:LYS:CG	2.28	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:467:ASP:O	1:B:468:VAL:C	2.59	0.45
1:B:278:GLU:C	1:B:280:ASN:N	2.73	0.45
1:A:391:ASP:HA	1:A:398:ARG:NH1	2.31	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:335:LYS:HE3	1:B:336:LYS:HZ3	1.82	0.45
1:A:276:SER:HB2	1:A:279:GLU:HB2	1.97	0.44
1:B:363:PHE:O	1:B:367:LYS:HB2	2.17	0.44
1:A:423:ASN:HD22	1:A:424:PRO:C	2.25	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:411:VAL:HG12	1:B:415:LEU:HD22	1.99	0.44
1:A:454:ASN:N	1:A:454:ASN:ND2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TYR:OH	1:B:362:MET:HE3	2.17	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:253:ILE:HD12	1:B:253:ILE:C	2.43	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:248:THR:O	1:A:249:LEU:C	2.61	0.43
1:A:358:TYR:C	1:A:361:PRO:HD2	2.42	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:B:335:LYS:C	1:B:337:LEU:H	2.26	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:430:LEU:C	1:A:432:GLY:H	2.26	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:A:350:ARG:NH1	1:A:359:ILE:HG13	2.34	0.42
1:B:286:GLU:O	1:B:287:MET:C	2.61	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:299:THR:C	1:B:301:ARG:N	2.77	0.42
1:B:447:MET:HE3	1:B:451:TRP:HB2	2.00	0.42
1:B:317:LEU:HG	2:D:5:LEU:HD11	2.00	0.42
1:A:302:LEU:O	1:A:303:PRO:C	2.62	0.42
1:B:292:VAL:O	1:B:293:GLN:C	2.63	0.42
1:B:292:VAL:HG12	1:B:293:GLN:N	2.34	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:317:LEU:O	1:B:318:LYS:C	2.63	0.42
1:A:325:MET:HE3	1:A:325:MET:HB3	1.96	0.42
1:A:326:PHE:HD2	1:A:366:TYR:OH	2.03	0.42
1:B:346:GLU:CD	5:B:15:HOH:O	2.61	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:335:LYS:O	1:B:336:LYS:C	2.62	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: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:B:419:TYR:C	1:B:421:PRO:HD3	2.45	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:268:ASN:ND2	1:B:268:ASN:N	2.65	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:B:261:ARG:O	1:B:262:MET:C	2.62	0.41
1:B:452:ARG:O	1:B:453:VAL:HG12	2.20	0.41
2:D:11:LYS:O	2:D:12:ASP:CG	2.64	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: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:A:290:SER:O	1:A:291:HIS:C	2.63	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:A:355:SER:C	1:A:357:GLU:N	2.78	0.40
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:A:403:LYS:O	1:A:407:PRO:CD	2.70	0.40
1:B:358:TYR:CZ	1:B:362:MET:HE3	2.56	0.40
1:A:390:PRO:HA	1:A:395:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:287:MET:O	1:A:288:ALA:C	2.64	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
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

5.3.1 Protein backbone

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%)	0	1
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

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Mol	Chain	Res	Type
1	A	424	PRO
1	B	303	PRO
1	B	305	PHE
1	B	321	ALA
1	B	337	LEU
1	B	373	LYS
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 ⓘ

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%)	189 (90%)	20 (10%)	8	26
1	B	209/210 (100%)	183 (88%)	26 (12%)	4	15
2	C	10/11 (91%)	10 (100%)	0	100	100
2	D	11/11 (100%)	9 (82%)	2 (18%)	2	6
2	E	10/11 (91%)	9 (90%)	1 (10%)	7	24
All	All	449/453 (99%)	400 (89%)	49 (11%)	6	20

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	LEU
1	A	299	THR
1	A	300	LYS
1	A	302	LEU
1	A	306	GLN
1	A	328	ARG
1	A	341	HIS
1	A	344	LEU
1	A	351	LYS
1	A	354	ILE
1	A	359	ILE
1	A	371	GLU
1	A	376	GLN
1	A	385	ILE
1	A	403	LYS
1	A	406	GLU
1	A	409	LEU
1	A	423	ASN
1	A	434	LEU
1	A	468	VAL
1	B	242	LEU
1	B	261	ARG
1	B	269	LYS
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

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Mol	Chain	Res	Type
1	B	337	LEU
1	B	338	PRO
1	B	354	ILE
1	B	377	GLU
1	B	388	LEU
1	B	405	GLN
1	B	415	LEU
1	B	422	GLU
1	B	433	ARG
1	B	447	MET
1	B	449	MET
1	B	452	ARG
1	B	453	VAL
1	B	465	ILE
1	B	467	ASP
2	D	1	GLU
2	D	5	LEU
2	E	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	260	GLN
1	A	264	GLN
1	A	293	GLN
1	A	306	GLN
1	A	310	HIS
1	A	376	GLN
1	A	423	ASN
1	A	425	GLN
1	A	442	HIS
1	A	444	HIS
1	A	454	ASN
1	B	264	GLN
1	B	268	ASN
1	B	280	ASN
1	B	310	HIS
1	B	313	GLN
1	B	334	ASN
1	B	341	HIS
1	B	376	GLN

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Mol	Chain	Res	Type
1	B	420	GLN
1	B	423	ASN
1	B	426	HIS
1	B	441	ASN
1	B	456	HIS
2	D	2	ASN
2	E	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 oligosaccharides 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
3	CHC	A	1001	-	33,33,33	3.67	19 (57%)	52,52,52	1.77	11 (21%)
4	IU5	B	1002	-	30,30,31	2.57	15 (50%)	47,47,49	1.52	9 (19%)

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
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(°)	Ideal(°)
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
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:

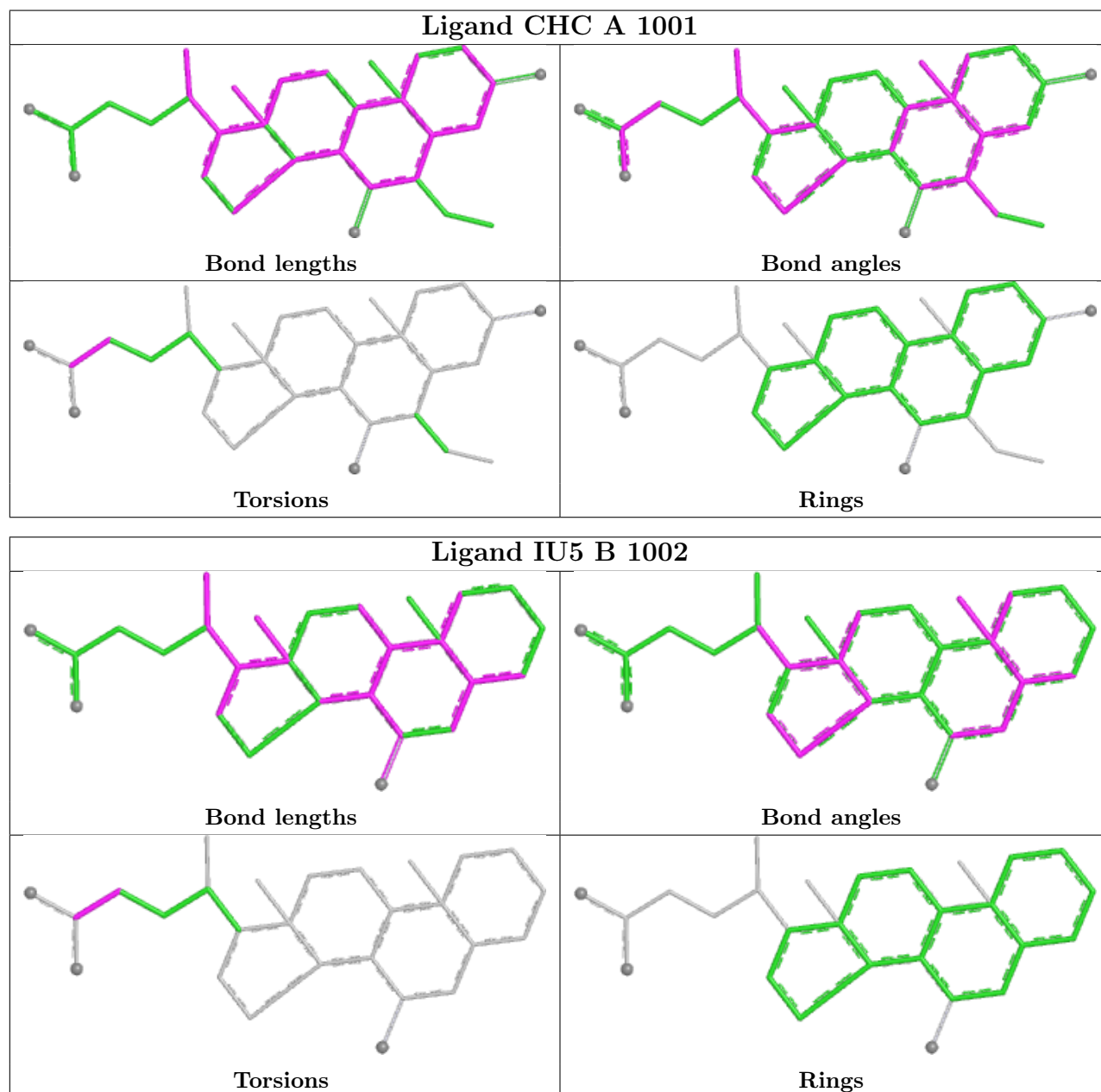
Mol	Chain	Res	Type	Atoms
4	B	1002	IU5	C22-C23-C24-O4A
4	B	1002	IU5	C22-C23-C24-O4
3	A	1001	CHC	C22-C23-C24-OT2
3	A	1001	CHC	C22-C23-C24-OT1

There are no ring outliers.

2 monomers are involved in 7 short contacts:

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	229/229 (100%)	0.24	9 (3%)	43	35	11, 78, 152, 189	8 (3%)
1	B	229/229 (100%)	0.15	9 (3%)	43	35	33, 69, 137, 183	1 (0%)
2	C	12/12 (100%)	0.34	0	100	100	56, 68, 104, 187	0
2	D	12/12 (100%)	0.34	0	100	100	46, 70, 86, 105	0
2	E	12/12 (100%)	0.10	0	100	100	62, 92, 124, 177	0
All	All	494/494 (100%)	0.20	18 (3%)	46	38	11, 73, 150, 189	9 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	THR	6.1
1	B	468	VAL	3.2
1	B	348	ARG	2.9
1	B	341	HIS	2.8
1	A	241	GLU	2.6
1	B	253	ILE	2.6
1	A	449	MET	2.5
1	A	351	LYS	2.4
1	A	419	TYR	2.4
1	B	262	MET	2.3
1	A	372	LEU	2.3
1	A	275	PHE	2.2
1	A	468	VAL	2.2
1	B	442	HIS	2.2
1	B	240	THR	2.1
1	A	338	PRO	2.1
1	B	263	PRO	2.0
1	B	419	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

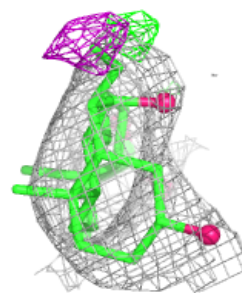
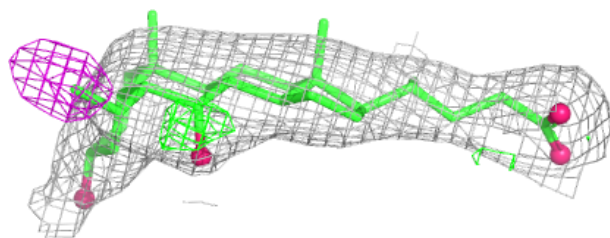
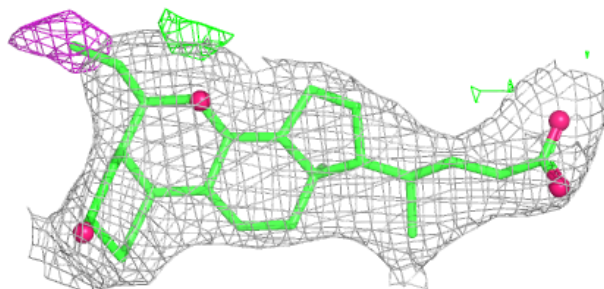
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CHC	A	1001	30/30	0.87	0.14	23,60,63,65	0
4	IU5	B	1002	27/28	0.90	0.12	40,43,49,52	0

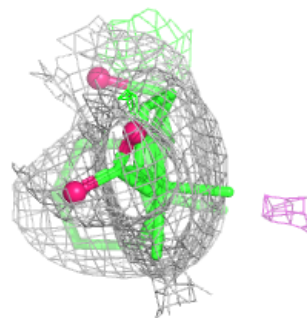
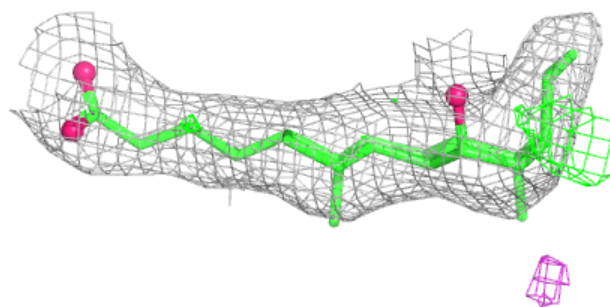
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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