Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 12:39 am BST

PDB ID	:	1GWX
Title	:	MOLECULAR RECOGNITION OF FATTY ACIDS BY PEROXISOME PROLIFERATOR-ACTIVATED RECEPTORS
Authors	:	Xu, H.E.; Lambert, M.H.; Montana, V.G.; Park, D.J.; Blanchard, S.; Brown, P.; Sternbach, D.; Lehmann, J.; Bruce, G.W.; Willson, T.M.; Kliewer, S.A.; Milburn, M.V.
Deposited on	:	1999-03-17
Resolution	:	2.50 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.

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

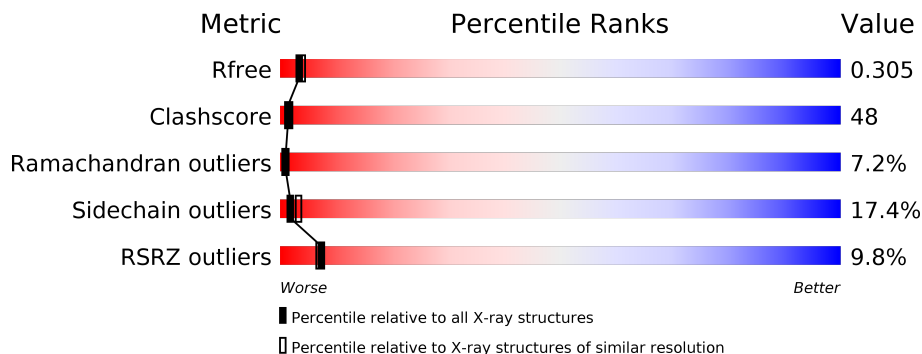|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	Percentile Ranks	Value
Rfree		0.305
Clashscore		48
Ramachandran outliers		7.2%
Sidechain outliers		17.4%
RSRZ outliers		9.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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.

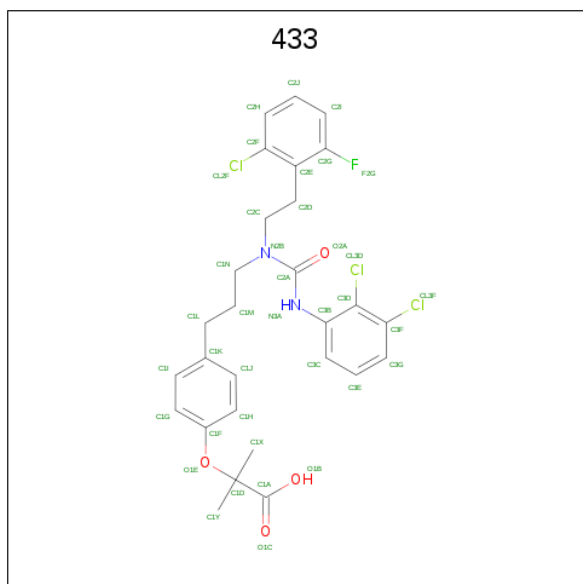| Mol	Chain	Length	Quality of chain
1	A	271	9% 37% 48% 14% •
1	B	271	11% 38% 48% 13% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4493 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 PROTEIN (PPAR-DELTA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	1
			2172	1405	368	389	10			
1	B	271	Total	C	N	O	S	0	0	0
			2158	1396	362	390	10			

- Molecule 2 is 2-(4-{3-[1-[2-(2-CHLORO-6-FLUORO-PHENYL)-ETHYL]-3-(2,3-DICHLORO-PHENYL)-UREIDO]-PROPYL}-PHENOXY)-2-METHYL-PROPIONIC ACID (three-letter code: 433) (formula: $C_{28}H_{28}Cl_3FN_2O_4$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			38	28	3	1	2	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			38	28	3	1	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	36	Total 36	O 36	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 a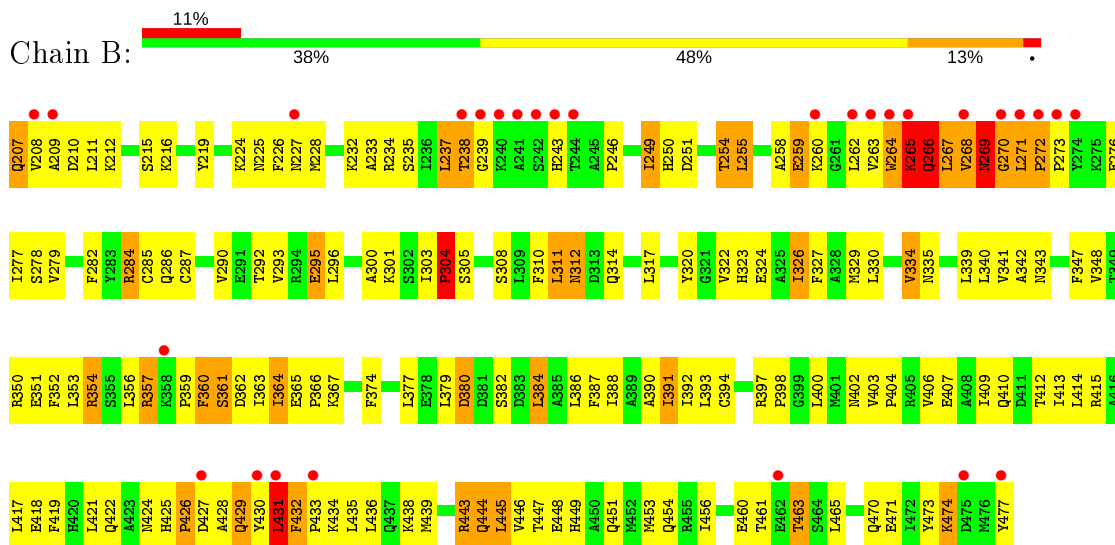nnotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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: PROTEIN (PPAR-DELTA)

Chain A:

- Molecule 1: PROTEIN (PPAR-DELTA)

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.25Å 94.90Å 96.20Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 13.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	73.4 (8.00-2.50) 73.0 (13.18-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$<I/\sigma(I)>$ [1]	2.39 (at 2.50Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.246 , 0.303 0.248 , 0.305	Depositor DCC
R_{free} test set	1786 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 60.3	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4493	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 433

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	0.47	0/2219	0.68	0/3001
1	B	0.42	0/2205	0.66	0/2986
All	All	0.44	0/4424	0.67	0/5987

There are no bond length outliers.

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	2172	0	2218	209	0
1	B	2158	0	2173	220	0
2	A	38	0	27	7	0
2	B	38	0	27	9	0
3	A	51	0	0	1	0
3	B	36	0	0	1	0
All	All	4493	0	4445	426	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 (426) 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:266:GLN:CD	1:A:267:LEU:H	1.59	1.04
1:B:363:ILE:HD11	1:B:453:MET:HE2	1.42	1.00
1:B:249:ILE:O	1:B:254:THR:HG21	1.62	0.98
1:B:322:VAL:O	1:B:326:ILE:HG22	1.63	0.97
1:A:236:ILE:HA	1:A:243:HIS:NE2	1.81	0.95
1:B:310:PHE:HB3	1:B:312:ASN:HD21	1.32	0.94
1:B:431:LEU:O	1:B:433:PRO:HD2	1.69	0.92
1:B:312:ASN:H	1:B:312:ASN:HD22	1.11	0.92
1:A:245:ALA:HB3	1:B:209:ALA:HB3	1.50	0.90
1:A:455:ARG:O	1:A:459:THR:HG22	1.72	0.90
1:A:271:LEU:O	1:A:276:GLU:HA	1.74	0.87
1:B:310:PHE:HB3	1:B:312:ASN:ND2	1.90	0.86
1:B:421:LEU:HB3	1:B:431:LEU:HD23	1.59	0.85
1:B:465:LEU:HD23	1:B:470:GLN:HE21	1.43	0.84
1:A:297:THR:O	1:A:301:LYS:HG3	1.78	0.84
1:B:277:ILE:HG23	1:B:278:SER:H	1.44	0.83
1:A:348:VAL:HG11	2:A:1:433:CL3F	2.15	0.83
1:A:270:GLY:O	1:A:271:LEU:HD13	1.78	0.83
1:A:275:LYS:HE3	1:A:280:HIS:HA	1.62	0.82
1:B:430:TYR:HA	1:B:434:LYS:HD3	1.59	0.82
1:B:431:LEU:H	1:B:431:LEU:HD12	1.45	0.81
1:B:250:HIS:HA	1:B:352:PHE:HB2	1.61	0.81
1:B:312:ASN:N	1:B:312:ASN:HD22	1.80	0.80
1:A:268:VAL:HG22	1:A:269:ASN:H	1.47	0.79
1:B:418:GLU:HA	1:B:432:PHE:CZ	2.17	0.79
1:A:296:LEU:HD22	1:A:392:ILE:HD11	1.64	0.78
1:A:215:SER:OG	1:A:386:LEU:HD11	1.83	0.78
1:B:251:ASP:OD1	1:B:254:THR:HG22	1.84	0.76
1:B:424:ASN:HD22	1:B:425:HIS:CE1	2.03	0.76
1:B:286:GLN:O	1:B:290:VAL:HG23	1.86	0.76
1:A:357:ARG:HH12	1:A:460:GLU:CD	1.90	0.76
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.68	0.74
1:B:269:ASN:ND2	1:B:271:LEU:HD21	2.02	0.74
1:B:269:ASN:HD21	1:B:271:LEU:HD21	1.50	0.74
1:B:460:GLU:HB3	1:B:463:THR:HG23	1.70	0.73
1:A:430:TYR:O	1:A:434:LYS:HB2	1.89	0.73
1:B:430:TYR:HA	1:B:434:LYS:CD	2.20	0.72
1:A:391:ILE:HD12	1:A:391:ILE:O	1.90	0.72
1:B:305:SER:O	1:B:308:SER:HB2	1.90	0.72
1:B:460:GLU:HB3	1:B:463:THR:CG2	2.20	0.72
1:B:339:LEU:HG	1:B:340:LEU:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:THR:HG22	1:B:239:GLY:N	2.05	0.71
1:A:267:LEU:HD11	1:A:284:ARG:HG2	1.72	0.70
1:A:275:LYS:HG2	1:A:279:VAL:HG12	1.74	0.70
1:A:321:GLY:O	1:A:391:ILE:HD11	1.90	0.70
1:B:334:VAL:HG13	1:B:335:ASN:H	1.56	0.70
1:A:271:LEU:HB3	1:A:277:ILE:N	2.07	0.70
1:B:330:LEU:HD13	2:B:2:433:CL2F	2.28	0.70
1:A:266:GLN:NE2	1:A:267:LEU:H	1.88	0.70
1:A:351:GLU:HG3	1:A:352:PHE:N	2.05	0.70
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.74	0.70
1:B:320:TYR:HB3	1:B:397:ARG:HD2	1.73	0.70
1:B:473:TYR:O	1:B:474:LYS:HB3	1.92	0.70
1:A:271:LEU:CA	1:A:276:GLU:HA	2.21	0.69
1:A:266:GLN:HB3	1:A:267:LEU:HD23	1.75	0.69
1:B:387:PHE:O	1:B:391:ILE:HG22	1.93	0.69
1:B:260:LYS:HE2	1:B:268:VAL:HB	1.74	0.69
1:A:266:GLN:CD	1:A:267:LEU:N	2.42	0.68
1:B:207:GLN:HG3	1:B:210:ASP:HB3	1.74	0.68
1:B:272:PRO:HB2	1:B:273:PRO:CD	2.24	0.68
1:B:323:HIS:HA	1:B:326:ILE:CG2	2.23	0.68
1:B:268:VAL:O	1:B:269:ASN:HB2	1.94	0.68
1:B:310:PHE:CB	1:B:312:ASN:HD21	2.05	0.68
1:B:259:GLU:OE2	1:B:284:ARG:NH1	2.27	0.67
1:B:334:VAL:CG1	1:B:335:ASN:N	2.57	0.67
1:B:312:ASN:H	1:B:312:ASN:ND2	1.89	0.67
1:B:430:TYR:O	1:B:434:LYS:HB2	1.93	0.67
1:A:236:ILE:HA	1:A:243:HIS:CE1	2.29	0.67
1:A:267:LEU:O	1:A:268:VAL:HG12	1.95	0.67
1:B:266:GLN:HG2	1:B:284:ARG:NH2	2.09	0.67
1:A:268:VAL:HA	1:A:280:HIS:HE1	1.59	0.67
1:B:377:LEU:HD11	1:B:438:LYS:HD2	1.77	0.67
1:A:387:PHE:O	1:A:391:ILE:HG23	1.95	0.66
1:B:354:ARG:HB3	1:B:354:ARG:NH1	2.10	0.66
1:B:271:LEU:HD13	1:B:277:ILE:HA	1.77	0.66
1:A:271:LEU:C	1:A:276:GLU:HA	2.14	0.66
1:A:233:ALA:O	1:A:237:LEU:HD12	1.96	0.66
1:A:258:ALA:HA	1:A:262:LEU:HD13	1.76	0.66
1:B:334:VAL:HG13	1:B:335:ASN:N	2.11	0.65
1:B:215:SER:HA	1:B:386:LEU:HD21	1.78	0.65
1:B:265:LYS:HE2	1:B:265:LYS:O	1.97	0.65
1:B:415:ARG:O	1:B:418:GLU:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:MET:O	1:A:456:ILE:HG22	1.97	0.64
1:B:233:ALA:O	1:B:237:LEU:HD23	1.97	0.64
1:A:249:ILE:HD12	1:A:348:VAL:HG22	1.78	0.64
1:B:300:ALA:HA	1:B:303:ILE:HD13	1.78	0.64
1:B:356:LEU:HB2	1:B:361:SER:HB3	1.79	0.64
1:A:259:GLU:OE2	1:A:284:ARG:NH1	2.31	0.64
1:B:324:GLU:HB2	1:B:391:ILE:CD1	2.27	0.64
1:B:431:LEU:H	1:B:431:LEU:CD1	2.04	0.64
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.27	0.64
1:A:267:LEU:CD1	1:A:284:ARG:HG2	2.27	0.64
1:A:374:PHE:O	1:A:377:LEU:HD13	1.98	0.63
1:A:228:MET:HE1	1:A:232:LYS:HG2	1.81	0.63
1:A:259:GLU:CD	1:A:284:ARG:HH12	2.01	0.63
1:A:271:LEU:O	1:A:276:GLU:CA	2.47	0.63
1:A:207:GLN:HB2	1:A:209:ALA:O	1.98	0.63
1:B:431:LEU:O	1:B:432:PHE:HB2	1.97	0.63
1:A:244:THR:HA	1:B:208:VAL:HG23	1.81	0.62
1:B:418:GLU:HA	1:B:432:PHE:HZ	1.64	0.62
1:A:425:HIS:HB3	1:A:428:ALA:HB2	1.82	0.62
1:B:249:ILE:O	1:B:250:HIS:ND1	2.31	0.62
1:A:402:ASN:HD22	1:A:404:PRO:HD2	1.64	0.61
1:B:282:PHE:HE1	1:B:453:MET:HE1	1.65	0.61
1:A:312:ASN:O	1:A:316:THR:HG23	1.99	0.61
1:B:432:PHE:O	1:B:436:LEU:HB2	2.01	0.61
1:B:471:GLU:OE1	1:B:474:LYS:HE2	2.00	0.61
1:A:289:THR:O	1:A:293:VAL:HG23	2.00	0.60
1:A:243:HIS:O	1:B:207:GLN:HA	2.00	0.60
1:A:262:LEU:HD12	1:A:262:LEU:N	2.16	0.60
1:A:449:HIS:O	1:A:453:MET:HG2	2.01	0.60
1:B:277:ILE:HG23	1:B:278:SER:N	2.13	0.60
1:B:348:VAL:HG11	2:B:2:433:CL3F	2.38	0.60
1:A:228:MET:SD	1:A:232:LYS:HE3	2.41	0.60
1:B:237:LEU:HD21	1:B:340:LEU:HD13	1.82	0.60
1:A:403:VAL:HG13	1:A:404:PRO:HD3	1.82	0.60
1:B:354:ARG:HB3	1:B:354:ARG:HH11	1.65	0.60
1:B:266:GLN:CG	1:B:284:ARG:HH22	2.14	0.60
1:A:324:GLU:CB	1:A:391:ILE:HD13	2.32	0.59
1:A:445:LEU:O	1:A:448:GLU:HG3	2.01	0.59
1:B:249:ILE:HG22	1:B:250:HIS:N	2.15	0.59
1:A:435:LEU:O	1:A:439:MET:HG3	2.02	0.59
1:B:424:ASN:HD22	1:B:425:HIS:HE1	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:N	1:B:431:LEU:HD12	2.15	0.59
1:B:397:ARG:HB2	1:B:400:LEU:HD22	1.84	0.59
1:A:268:VAL:O	1:A:269:ASN:CB	2.50	0.59
1:B:363:ILE:CD1	1:B:453:MET:HE2	2.26	0.59
1:B:377:LEU:HD22	1:B:430:TYR:HB2	1.84	0.58
1:B:226:PHE:HZ	1:B:296:LEU:HD23	1.66	0.58
1:A:243:HIS:C	1:B:207:GLN:HB3	2.23	0.58
1:A:264:TRP:HB3	1:A:284:ARG:NH2	2.18	0.58
1:B:271:LEU:HB3	1:B:276:GLU:C	2.24	0.58
1:B:473:TYR:O	1:B:474:LYS:CB	2.52	0.57
1:B:279:VAL:HG22	1:B:360:PHE:CZ	2.40	0.57
1:A:270:GLY:C	1:A:271:LEU:HD13	2.25	0.57
1:B:249:ILE:C	1:B:254:THR:HG21	2.24	0.57
1:A:273:PRO:O	1:A:275:LYS:N	2.37	0.57
1:B:388:ILE:O	1:B:391:ILE:HG23	2.04	0.57
1:B:228:MET:HE3	1:B:233:ALA:HA	1.85	0.57
1:B:357:ARG:NH2	1:B:460:GLU:OE2	2.36	0.57
1:B:379:LEU:HD11	1:B:435:LEU:HD11	1.87	0.57
1:B:384:LEU:O	1:B:388:ILE:HG12	2.04	0.57
1:B:451:GLN:O	1:B:454:GLN:HG2	2.04	0.57
1:A:411:ASP:CG	1:A:415:ARG:HH21	2.08	0.57
1:B:208:VAL:O	1:B:208:VAL:HG12	2.03	0.57
1:B:250:HIS:NE2	1:B:251:ASP:OD2	2.38	0.56
1:A:259:GLU:O	1:A:263:VAL:HA	2.06	0.56
1:A:272:PRO:N	1:A:273:PRO:HD2	2.21	0.56
1:B:387:PHE:CE2	1:B:435:LEU:HG	2.39	0.56
1:A:266:GLN:C	1:A:267:LEU:HD23	2.25	0.56
1:A:447:THR:O	1:A:451:GLN:HG3	2.05	0.56
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.87	0.56
1:A:324:GLU:HB2	1:A:391:ILE:HD13	1.87	0.56
1:A:387:PHE:CE1	1:A:435:LEU:HD22	2.40	0.56
1:A:208:VAL:HG23	1:A:419:PHE:CE2	2.41	0.56
1:A:271:LEU:HD22	1:A:271:LEU:N	2.21	0.56
1:B:430:TYR:CE2	1:B:431:LEU:HG	2.41	0.56
1:B:465:LEU:HD23	1:B:470:GLN:HG2	1.87	0.55
1:A:425:HIS:HB3	1:A:428:ALA:CB	2.36	0.55
1:B:410:GLN:O	1:B:413:ILE:HB	2.07	0.55
1:A:268:VAL:HA	1:A:280:HIS:CE1	2.41	0.55
1:A:211:LEU:HD11	1:A:412:THR:HG23	1.87	0.55
1:B:312:ASN:N	1:B:312:ASN:ND2	2.50	0.55
1:A:466:HIS:HB3	1:A:469:LEU:HD22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HB2	1:A:332:SER:HB3	1.89	0.55
1:B:465:LEU:CD2	1:B:470:GLN:HE21	2.17	0.55
2:A:1:433:H1G1	2:A:1:433:C1A	2.37	0.54
1:A:276:GLU:OE2	1:A:357:ARG:NH2	2.32	0.54
1:B:232:LYS:O	1:B:235:SER:HB3	2.07	0.54
1:B:324:GLU:HB2	1:B:391:ILE:HD11	1.89	0.54
1:B:430:TYR:HA	1:B:434:LYS:CG	2.37	0.54
1:B:209:ALA:HA	1:B:212:LYS:HB2	1.88	0.54
1:A:379:LEU:HD11	1:A:435:LEU:HD21	1.90	0.54
1:B:259:GLU:HG2	1:B:269:ASN:HA	1.90	0.54
1:B:360:PHE:O	1:B:362:ASP:N	2.34	0.54
1:A:271:LEU:HA	1:A:276:GLU:HA	1.90	0.54
1:B:264:TRP:HB3	1:B:284:ARG:HH22	1.73	0.54
1:B:419:PHE:O	1:B:422:GLN:HB2	2.08	0.54
1:B:292:THR:HA	1:B:295:GLU:HG3	1.90	0.54
1:B:365:GLU:N	1:B:366:PRO:HD2	2.21	0.53
1:A:306:PHE:CE2	1:A:314:GLN:HG2	2.44	0.53
1:B:324:GLU:HB2	1:B:391:ILE:HD13	1.91	0.53
1:A:429:GLN:HE21	1:A:429:GLN:C	2.11	0.53
1:A:476:MET:HG2	1:A:477:TYR:N	2.24	0.53
1:B:387:PHE:CD2	1:B:435:LEU:HG	2.44	0.53
1:B:209:ALA:HA	1:B:212:LYS:CB	2.38	0.53
1:A:432:PHE:HB3	1:A:433:PRO:CD	2.39	0.53
1:B:418:GLU:CA	1:B:432:PHE:HZ	2.21	0.53
1:A:353:LEU:HD21	2:A:1:433:CL3F	2.46	0.52
1:A:214:PHE:CZ	1:A:412:THR:HG22	2.45	0.52
1:B:268:VAL:O	1:B:269:ASN:CB	2.58	0.52
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.37	0.52
1:A:217:HIS:HE1	1:A:302:SER:O	1.92	0.52
1:A:330:LEU:O	1:A:330:LEU:HD22	2.09	0.52
1:B:340:LEU:HD12	1:B:347:PHE:HD1	1.73	0.52
1:B:456:ILE:O	1:B:460:GLU:HB2	2.10	0.52
1:A:250:HIS:CE1	1:A:251:ASP:OD2	2.63	0.52
1:B:430:TYR:CA	1:B:434:LYS:HD3	2.34	0.52
1:B:271:LEU:HD13	1:B:277:ILE:CA	2.40	0.52
1:A:280:HIS:HE2	1:A:284:ARG:NH1	2.08	0.51
1:B:225:ASN:O	1:B:295:GLU:HB3	2.10	0.51
1:B:435:LEU:O	1:B:439:MET:HG3	2.10	0.51
1:B:418:GLU:HA	1:B:432:PHE:CE1	2.45	0.51
1:B:421:LEU:HD22	1:B:430:TYR:OH	2.10	0.51
1:A:247:PHE:CD2	1:A:262:LEU:HG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:HG2	1:A:474:LYS:O	2.09	0.51
1:B:264:TRP:CZ2	1:B:342:ALA:HB2	2.46	0.51
1:A:271:LEU:HD12	1:A:276:GLU:O	2.11	0.51
1:B:266:GLN:O	1:B:267:LEU:HB3	2.10	0.51
1:B:284:ARG:HG2	2:B:2:433:C3E	2.40	0.51
1:A:393:LEU:O	1:A:410:GLN:HB2	2.10	0.51
1:B:303:ILE:HG23	1:B:304:PRO:HD2	1.92	0.51
1:B:421:LEU:HD12	1:B:431:LEU:HB3	1.93	0.51
1:A:449:HIS:NE2	2:A:1:433:O1C	2.43	0.51
1:A:240:LYS:HG2	1:A:240:LYS:O	2.09	0.51
1:B:470:GLN:O	1:B:473:TYR:O	2.29	0.51
1:A:230:LYS:CB	1:A:332:SER:HB3	2.40	0.51
1:B:351:GLU:HA	1:B:354:ARG:HG3	1.92	0.51
1:B:270:GLY:C	1:B:271:LEU:HD23	2.31	0.50
1:A:296:LEU:HD13	1:A:322:VAL:HG22	1.93	0.50
1:A:334:VAL:HG13	1:A:335:ASN:N	2.27	0.50
1:A:269:ASN:CG	1:A:270:GLY:N	2.64	0.50
1:B:271:LEU:N	1:B:271:LEU:HD23	2.27	0.50
1:B:323:HIS:HE2	2:B:2:433:C1A	2.23	0.50
1:A:245:ALA:CB	1:B:209:ALA:HB3	2.32	0.50
1:B:359:PRO:HG2	1:B:360:PHE:CD1	2.46	0.50
1:B:429:GLN:C	1:B:431:LEU:HD12	2.31	0.50
1:B:410:GLN:O	1:B:413:ILE:N	2.44	0.50
1:A:209:ALA:O	1:A:210:ASP:CB	2.60	0.50
1:A:222:TYR:CE1	1:A:381:ASP:HB3	2.46	0.50
1:B:353:LEU:HD21	2:B:2:433:CL3D	2.49	0.50
1:B:266:GLN:HG2	1:B:284:ARG:HH22	1.72	0.50
1:A:247:PHE:HD2	1:A:262:LEU:HG	1.75	0.50
1:B:348:VAL:HG13	1:B:352:PHE:HD2	1.76	0.50
1:A:236:ILE:O	1:A:243:HIS:HE1	1.95	0.50
1:A:268:VAL:HG22	1:A:269:ASN:N	2.24	0.50
1:A:368:PHE:O	1:A:372:VAL:HG23	2.12	0.49
1:A:275:LYS:HG2	1:A:279:VAL:CG1	2.41	0.49
1:B:417:LEU:O	1:B:421:LEU:HG	2.13	0.49
1:B:226:PHE:CE1	1:B:295:GLU:HB2	2.46	0.49
1:B:403:VAL:O	1:B:407:GLU:HG3	2.12	0.49
1:A:277:ILE:O	1:A:280:HIS:HB3	2.12	0.49
1:A:357:ARG:NH1	1:A:460:GLU:OE2	2.39	0.49
1:B:267:LEU:O	1:B:269:ASN:N	2.40	0.49
1:B:350:ARG:O	1:B:354:ARG:HG2	2.12	0.49
1:B:249:ILE:HD12	1:B:249:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:CA	1:A:280:HIS:HE1	2.24	0.49
1:A:263:VAL:O	1:A:264:TRP:CB	2.61	0.49
1:A:335:ASN:HD22	1:A:347:PHE:HZ	1.61	0.49
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.78	0.48
1:B:304:PRO:HA	3:B:509:HOH:O	2.13	0.48
1:B:323:HIS:HA	1:B:326:ILE:HG22	1.94	0.48
1:A:417:LEU:O	1:A:421:LEU:HG	2.14	0.48
1:A:411:ASP:O	1:A:415:ARG:HB2	2.14	0.48
1:A:476:MET:CG	1:A:477:TYR:N	2.76	0.48
1:B:237:LEU:HD22	1:B:237:LEU:N	2.27	0.48
1:B:414:LEU:HD22	1:B:436:LEU:HD21	1.95	0.48
1:B:374:PHE:HD2	1:B:438:LYS:HD3	1.79	0.48
1:A:271:LEU:O	1:A:275:LYS:O	2.31	0.48
1:A:472:ILE:HG22	1:A:476:MET:CE	2.44	0.48
1:B:380:ASP:C	1:B:380:ASP:OD1	2.52	0.48
1:A:419:PHE:O	1:A:422:GLN:HB2	2.13	0.48
1:B:323:HIS:HA	1:B:326:ILE:HG23	1.96	0.48
1:A:377:LEU:N	1:A:377:LEU:HD12	2.28	0.48
1:B:390:ALA:HA	1:B:413:ILE:HG21	1.96	0.48
1:A:270:GLY:C	1:A:271:LEU:HD22	2.34	0.47
1:A:306:PHE:HD1	1:A:393:LEU:HD21	1.78	0.47
1:A:324:GLU:HB3	1:A:391:ILE:HD13	1.95	0.47
1:A:335:ASN:OD1	1:A:336:LYS:N	2.47	0.47
1:A:418:GLU:HB2	1:A:432:PHE:CD1	2.49	0.47
1:A:208:VAL:HG13	1:A:209:ALA:N	2.29	0.47
1:A:235:SER:O	1:A:238:THR:HG22	2.14	0.47
1:B:296:LEU:HD12	1:B:322:VAL:HG22	1.96	0.47
1:A:250:HIS:CD2	1:A:254:THR:HG21	2.49	0.47
1:A:374:PHE:CD1	1:A:438:LYS:HG2	2.49	0.47
1:A:247:PHE:CZ	1:B:212:LYS:NZ	2.82	0.47
1:A:267:LEU:HD11	1:A:284:ARG:CG	2.43	0.47
1:B:265:LYS:C	1:B:265:LYS:HE2	2.33	0.47
1:B:394:CYS:O	1:B:397:ARG:HG2	2.15	0.47
1:A:326:ILE:HG23	2:A:1:433:CL2F	2.52	0.47
1:A:411:ASP:OD2	1:A:415:ARG:NH2	2.40	0.47
1:A:418:GLU:HB2	1:A:432:PHE:CE1	2.50	0.47
1:A:472:ILE:O	1:A:476:MET:HE2	2.14	0.47
1:B:301:LYS:NZ	1:B:314:GLN:HE22	2.12	0.47
1:B:246:PRO:HB2	1:B:347:PHE:HB2	1.96	0.47
1:B:430:TYR:CD2	1:B:431:LEU:HG	2.50	0.47
1:A:268:VAL:O	1:A:269:ASN:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:THR:HG22	1:B:239:GLY:H	1.78	0.47
1:A:217:HIS:CE1	1:A:302:SER:O	2.67	0.47
1:A:331:ALA:HA	1:A:371:ALA:HB1	1.95	0.47
1:A:419:PHE:HA	1:A:422:GLN:CG	2.45	0.47
1:B:264:TRP:HB3	1:B:284:ARG:NH2	2.30	0.47
1:B:432:PHE:O	1:B:436:LEU:N	2.42	0.47
1:B:207:GLN:N	1:B:211:LEU:HD22	2.29	0.46
1:B:276:GLU:OE2	1:B:357:ARG:NH1	2.43	0.46
1:A:425:HIS:N	1:A:426:PRO:HD3	2.31	0.46
1:B:216:LYS:O	1:B:219:TYR:HB3	2.15	0.46
1:A:271:LEU:HD12	1:A:276:GLU:C	2.35	0.46
1:A:219:TYR:CE1	1:A:223:LEU:HD11	2.50	0.46
1:A:258:ALA:CA	1:A:262:LEU:HD13	2.46	0.46
1:A:264:TRP:CB	1:A:284:ARG:NH2	2.77	0.46
1:A:247:PHE:HD2	1:A:262:LEU:CG	2.28	0.46
1:A:291:GLU:O	1:A:295:GLU:HG3	2.15	0.46
1:A:297:THR:OG1	1:A:318:LEU:HD13	2.15	0.46
1:A:228:MET:HE3	1:A:233:ALA:N	2.31	0.46
1:A:334:VAL:CG1	1:A:335:ASN:N	2.79	0.46
1:B:421:LEU:CD1	1:B:431:LEU:HB3	2.45	0.46
1:A:264:TRP:HB3	1:A:284:ARG:HH21	1.80	0.46
1:A:271:LEU:HB3	1:A:276:GLU:C	2.36	0.46
1:A:240:LYS:HD3	1:A:240:LYS:H	1.80	0.45
1:A:419:PHE:HA	1:A:422:GLN:HG3	1.98	0.45
1:B:285:CYS:SG	2:B:2:433:H1N1	2.56	0.45
1:B:431:LEU:O	1:B:432:PHE:CB	2.65	0.45
1:B:300:ALA:O	1:B:303:ILE:HB	2.15	0.45
1:B:418:GLU:CA	1:B:432:PHE:CZ	2.94	0.45
1:A:263:VAL:O	1:A:264:TRP:CG	2.70	0.45
1:B:219:TYR:CD2	1:B:382:SER:HA	2.52	0.45
1:A:258:ALA:HA	1:A:262:LEU:CD1	2.44	0.45
1:A:324:GLU:HG3	1:A:446:VAL:HG21	1.98	0.45
1:B:255:LEU:HD12	1:B:277:ILE:HD11	1.98	0.45
1:B:324:GLU:CG	1:B:446:VAL:HG21	2.47	0.45
1:A:275:LYS:HD3	1:A:276:GLU:O	2.16	0.45
1:A:448:GLU:HB3	3:A:481:HOH:O	2.16	0.45
1:B:260:LYS:HE2	1:B:268:VAL:CB	2.45	0.45
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.99	0.45
1:B:277:ILE:CG2	1:B:278:SER:H	2.22	0.45
1:A:221:ALA:HB1	1:A:302:SER:HB2	1.99	0.45
1:A:335:ASN:ND2	1:A:338:GLY:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:TYR:CD1	1:A:476:MET:HE3	2.51	0.45
1:B:254:THR:O	1:B:258:ALA:HB2	2.17	0.45
1:B:377:LEU:HD11	1:B:438:LYS:CD	2.47	0.45
1:A:267:LEU:O	1:A:268:VAL:CG1	2.62	0.45
1:B:432:PHE:HB2	1:B:433:PRO:CD	2.47	0.45
1:A:262:LEU:O	1:A:263:VAL:HG23	2.17	0.44
1:B:363:ILE:HG12	1:B:363:ILE:O	2.16	0.44
1:B:391:ILE:HD12	1:B:397:ARG:NH2	2.31	0.44
1:A:418:GLU:O	1:A:422:GLN:HG2	2.18	0.44
1:A:246:PRO:HA	1:A:345:SER:O	2.17	0.44
1:A:340:LEU:HD22	1:A:344:GLY:HA2	1.98	0.44
1:B:272:PRO:CB	1:B:273:PRO:CD	2.95	0.44
1:B:327:PHE:CD2	1:B:445:LEU:HD13	2.52	0.44
1:B:390:ALA:CA	1:B:413:ILE:HG21	2.47	0.44
1:A:232:LYS:O	1:A:236:ILE:HG13	2.17	0.44
1:B:258:ALA:C	1:B:260:LYS:H	2.21	0.44
1:A:276:GLU:H	1:A:279:VAL:HB	1.82	0.44
1:A:460:GLU:HG3	1:A:463:THR:CG2	2.48	0.44
1:A:214:PHE:HE1	1:A:416:ALA:HB2	1.83	0.43
1:A:236:ILE:O	1:A:243:HIS:CE1	2.72	0.43
1:A:403:VAL:N	1:A:404:PRO:CD	2.81	0.43
1:B:380:ASP:OD1	1:B:382:SER:N	2.47	0.43
1:B:432:PHE:O	1:B:433:PRO:C	2.53	0.43
1:B:228:MET:HE1	1:B:340:LEU:HD23	2.00	0.43
1:B:249:ILE:O	1:B:250:HIS:CG	2.71	0.43
2:A:1:433:HN31	2:A:1:433:H1N1	1.60	0.43
1:A:234:ARG:HG2	1:A:234:ARG:NH1	2.34	0.43
1:A:335:ASN:ND2	1:A:337:ASP:H	2.16	0.43
1:A:445:LEU:C	1:A:445:LEU:HD23	2.39	0.43
1:A:268:VAL:O	1:A:269:ASN:CG	2.57	0.43
1:A:357:ARG:C	1:A:359:PRO:HD2	2.39	0.43
1:A:243:HIS:CG	1:A:244:THR:H	2.37	0.43
1:A:320:TYR:HB3	1:A:397:ARG:HD2	1.99	0.43
1:B:228:MET:CE	1:B:340:LEU:HD23	2.49	0.43
1:A:391:ILE:C	1:A:391:ILE:HD12	2.39	0.43
1:B:447:THR:HG23	1:B:477:TYR:OXT	2.19	0.43
1:B:397:ARG:HA	1:B:398:PRO:HD3	1.85	0.42
1:B:430:TYR:CG	1:B:431:LEU:N	2.87	0.42
1:B:209:ALA:C	1:B:212:LYS:H	2.22	0.42
1:B:393:LEU:HD13	1:B:409:ILE:CG2	2.49	0.42
1:A:240:LYS:N	1:A:240:LYS:HD3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:HIS:NE2	2:B:2:433:O1C	2.42	0.42
1:B:339:LEU:HD23	1:B:341:VAL:CG1	2.50	0.42
1:A:296:LEU:HD22	1:A:392:ILE:CD1	2.43	0.42
1:A:296:LEU:HD11	1:A:325:ALA:HB3	2.01	0.42
1:B:434:LYS:O	1:B:438:LYS:HG3	2.20	0.42
1:A:457:LYS:O	1:A:457:LYS:HG2	2.19	0.42
1:B:249:ILE:HA	1:B:254:THR:OG1	2.20	0.42
1:B:444:GLN:HB3	1:B:444:GLN:HE21	1.60	0.42
1:A:263:VAL:O	1:A:264:TRP:HB2	2.19	0.42
1:A:296:LEU:CD1	1:A:322:VAL:HG22	2.50	0.42
1:B:251:ASP:O	1:B:254:THR:HG23	2.20	0.42
1:B:324:GLU:HG2	1:B:446:VAL:HG21	2.02	0.42
1:A:215:SER:OG	1:A:386:LEU:HD21	2.20	0.41
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.68	0.41
1:B:391:ILE:HD12	1:B:397:ARG:HH21	1.84	0.41
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.92	0.41
1:B:435:LEU:HA	1:B:435:LEU:HD12	1.81	0.41
1:A:266:GLN:NE2	1:A:267:LEU:N	2.61	0.41
1:A:271:LEU:HA	1:A:275:LYS:O	2.19	0.41
1:A:359:PRO:O	1:A:363:ILE:HG23	2.20	0.41
1:A:471:GLU:OE1	1:A:471:GLU:HA	2.21	0.41
2:B:2:433:H1N1	2:B:2:433:HN31	1.69	0.41
1:A:255:LEU:O	1:A:259:GLU:HG2	2.21	0.41
1:B:296:LEU:HD12	1:B:322:VAL:CG2	2.50	0.41
1:B:356:LEU:HB2	1:B:361:SER:CB	2.48	0.41
1:A:267:LEU:N	1:A:267:LEU:HD23	2.36	0.41
1:A:429:GLN:O	1:A:431:LEU:N	2.48	0.41
1:A:284:ARG:HH11	1:A:284:ARG:CG	2.34	0.41
1:A:363:ILE:HA	1:A:452:MET:SD	2.61	0.41
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.86	0.41
1:B:303:ILE:HG21	1:B:393:LEU:HD11	2.02	0.41
1:B:353:LEU:HD21	2:B:2:433:CL3F	2.58	0.41
1:A:323:HIS:CE1	1:A:472:ILE:HG21	2.56	0.41
1:B:269:ASN:CG	1:B:270:GLY:H	2.24	0.41
1:B:364:ILE:HG12	1:B:364:ILE:H	1.71	0.41
1:B:386:LEU:HD13	1:B:417:LEU:HA	2.03	0.41
1:A:472:ILE:HG22	1:A:476:MET:HE1	2.02	0.41
1:A:310:PHE:O	1:A:313:ASP:N	2.52	0.40
1:A:323:HIS:HA	1:A:326:ILE:HB	2.02	0.40
1:A:416:ALA:O	1:A:420:HIS:N	2.53	0.40
1:B:207:GLN:CG	1:B:210:ASP:HB3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:MET:O	1:B:330:LEU:C	2.59	0.40
1:B:402:ASN:O	1:B:406:VAL:HG23	2.22	0.40
1:B:324:GLU:OE2	1:B:443:ARG:CD	2.69	0.40
1:A:267:LEU:C	1:A:268:VAL:O	2.59	0.40
1:B:293:VAL:HG13	1:B:322:VAL:HG21	2.02	0.40
1:B:465:LEU:HD23	1:B:470:GLN:NE2	2.23	0.40
1:A:286:GLN:HB3	2:A:1:433:H1Y1	2.03	0.40
1:A:351:GLU:HG3	1:A:352:PHE:H	1.79	0.40
1:B:224:LYS:HG3	1:B:224:LYS:O	2.20	0.40
1:A:255:LEU:HD13	1:A:277:ILE:CD1	2.51	0.40
1:A:274:TYR:CD2	1:A:274:TYR:N	2.87	0.40
1:B:317:LEU:HD22	1:B:392:ILE:O	2.21	0.40
1:A:268:VAL:HG13	1:A:269:ASN:N	2.37	0.40
1:B:238:THR:CG2	1:B:239:GLY:N	2.72	0.40
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.93	0.40
1:B:367:LYS:HG2	1:B:367:LYS:H	1.66	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	269/271 (99%)	230 (86%)	23 (9%)	16 (6%)	1	1
1	B	269/271 (99%)	218 (81%)	28 (10%)	23 (9%)	1	1
All	All	538/542 (99%)	448 (83%)	51 (10%)	39 (7%)	1	1

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	264	TRP

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Mol	Chain	Res	Type
1	A	266	GLN
1	A	268	VAL
1	A	269	ASN
1	A	429	GLN
1	B	238	THR
1	B	263	VAL
1	B	266	GLN
1	B	269	ASN
1	B	304	PRO
1	B	360	PHE
1	B	361	SER
1	B	426	PRO
1	B	432	PHE
1	B	474	LYS
1	A	263	VAL
1	A	265	LYS
1	A	274	TYR
1	B	237	LEU
1	B	268	VAL
1	B	343	ASN
1	B	428	ALA
1	B	429	GLN
1	B	461	THR
1	A	243	HIS
1	A	245	ALA
1	A	475	ASP
1	B	265	LYS
1	B	270	GLY
1	B	357	ARG
1	A	271	LEU
1	B	431	LEU
1	A	242	SER
1	A	430	TYR
1	B	427	ASP
1	B	272	PRO
1	B	249	ILE
1	A	359	PRO

5.3.2　Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/239 (100%)	191 (80%)	47 (20%)	1	2
1	B	233/239 (98%)	198 (85%)	35 (15%)	3	5
All	All	471/478 (98%)	389 (83%)	82 (17%)	2	3

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	214	PHE
1	A	223	LEU
1	A	224	LYS
1	A	240	LYS
1	A	250	HIS
1	A	253	GLU
1	A	262	LEU
1	A	263	VAL
1	A	265	LYS
1	A	266	GLN
1	A	267	LEU
1	A	269	ASN
1	A	271	LEU
1	A	274	TYR
1	A	275	LYS
1	A	277	ILE
1	A	287	CYS
1	A	289	THR
1	A	291	GLU
1	A	304	PRO
1	A	305	SER
1	A	322	VAL
1	A	330	LEU
1	A	334	VAL
1	A	335	ASN
1	A	339	LEU
1	A	356	LEU
1	A	357	ARG
1	A	361	SER
1	A	368	PHE

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Mol	Chain	Res	Type
1	A	391	ILE
1	A	400	LEU
1	A	402	ASN
1	A	403	VAL
1	A	417	LEU
1	A	424	ASN
1	A	429	GLN
1	A	431	LEU
1	A	434	LYS
1	A	447	THR
1	A	448	GLU
1	A	456	ILE
1	A	460	GLU
1	A	463	THR
1	A	469	LEU
1	A	470	GLN
1	B	207	GLN
1	B	227	ASN
1	B	234	ARG
1	B	243	HIS
1	B	254	THR
1	B	255	LEU
1	B	259	GLU
1	B	262	LEU
1	B	264	TRP
1	B	265	LYS
1	B	266	GLN
1	B	267	LEU
1	B	269	ASN
1	B	271	LEU
1	B	284	ARG
1	B	287	CYS
1	B	295	GLU
1	B	304	PRO
1	B	311	LEU
1	B	312	ASN
1	B	326	ILE
1	B	334	VAL
1	B	354	ARG
1	B	364	ILE
1	B	380	ASP
1	B	384	LEU

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Mol	Chain	Res	Type
1	B	391	ILE
1	B	412	THR
1	B	426	PRO
1	B	431	LEU
1	B	443	ARG
1	B	444	GLN
1	B	445	LEU
1	B	448	GLU
1	B	463	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	HIS
1	A	220	ASN
1	A	250	HIS
1	A	257	GLN
1	A	335	ASN
1	A	343	ASN
1	A	402	ASN
1	A	420	HIS
1	A	424	ASN
1	A	429	GLN
1	B	227	ASN
1	B	257	GLN
1	B	266	GLN
1	B	269	ASN
1	B	312	ASN
1	B	314	GLN
1	B	422	GLN
1	B	425	HIS
1	B	429	GLN
1	B	444	GLN
1	B	451	GLN
1	B	470	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 carbohydrates 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	#$|Z| > 2$
2	433	A	1	-	37,40,40	2.20	11 (29%)	51,56,56	3.32	25 (49%)
2	433	B	2	-	37,40,40	2.33	9 (24%)	51,56,56	3.41	25 (49%)

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	433	A	1	-	-	4/24/30/30	0/3/3/3
2	433	B	2	-	-	5/24/30/30	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	433	C3B-N3A	7.11	1.55	1.41
2	B	2	433	C2D-C2E	5.84	1.60	1.52
2	A	1	433	C2D-C2E	5.64	1.60	1.52
2	A	1	433	C3B-N3A	5.14	1.51	1.41
2	A	1	433	C2C-N2B	5.11	1.61	1.47
2	B	2	433	C2A-N3A	4.45	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	433	C2C-N2B	4.15	1.58	1.47
2	B	2	433	C1X-C1D	3.73	1.60	1.53
2	A	1	433	C3B-C3D	3.71	1.44	1.39
2	B	2	433	C3F-C3D	3.26	1.44	1.39
2	A	1	433	C2A-N2B	3.16	1.42	1.36
2	A	1	433	C1X-C1D	3.08	1.59	1.53
2	A	1	433	C2C-C2D	2.90	1.60	1.52
2	A	1	433	C1N-N2B	2.87	1.55	1.47
2	A	1	433	C2A-N3A	2.81	1.42	1.37
2	B	2	433	C3B-C3D	2.68	1.43	1.39
2	A	1	433	O1E-C1D	2.55	1.49	1.45
2	B	2	433	C2C-C2D	2.22	1.58	1.52
2	B	2	433	C1H-C1J	-2.18	1.34	1.38
2	A	1	433	C2I-C2G	2.10	1.42	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	433	C2D-C2C-N2B	13.65	136.25	112.64
2	B	2	433	C2D-C2C-N2B	11.41	132.37	112.64
2	B	2	433	C3D-C3F-CL3F	7.32	127.66	120.52
2	B	2	433	C3C-C3B-C3D	-6.59	113.84	118.88
2	B	2	433	C3B-N3A-C2A	6.31	141.86	125.52
2	A	1	433	C3C-C3B-C3D	-6.29	114.07	118.88
2	B	2	433	C2C-C2D-C2E	5.39	124.02	112.81
2	A	1	433	C1M-C1N-N2B	5.33	129.15	112.44
2	B	2	433	C1M-C1L-C1K	5.11	132.92	113.68
2	A	1	433	C3D-C3F-CL3F	5.07	125.47	120.52
2	B	2	433	C3B-C3D-CL3D	-5.07	115.82	119.52
2	A	1	433	C3B-N3A-C2A	5.03	138.53	125.52
2	B	2	433	N3A-C2A-N2B	5.02	121.64	115.89
2	A	1	433	N3A-C2A-N2B	5.01	121.63	115.89
2	A	1	433	C1M-C1L-C1K	4.86	131.97	113.68
2	B	2	433	C3G-C3F-CL3F	-4.79	108.79	118.41
2	A	1	433	C2C-C2D-C2E	4.63	122.45	112.81
2	B	2	433	C1Y-C1D-C1X	-4.30	103.31	110.14
2	A	1	433	C1D-O1E-C1F	4.28	128.28	121.04
2	A	1	433	O1E-C1D-C1X	4.23	122.66	105.72
2	B	2	433	C1X-C1D-C1A	-4.19	102.06	111.86
2	B	2	433	O1E-C1D-C1X	4.10	122.14	105.72
2	B	2	433	C1M-C1N-N2B	4.02	125.03	112.44
2	B	2	433	F2G-C2G-C2E	3.80	122.16	117.63

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Mol	Chain	Res	Type	Atoms	Z	Observed($^\circ$)	Ideal($^\circ$)
2	A	1	433	F2G-C2G-C2E	3.58	121.90	117.63
2	A	1	433	C1X-C1D-C1A	-3.56	103.53	111.86
2	A	1	433	C3G-C3F-CL3F	-3.52	111.34	118.41
2	B	2	433	O2A-C2A-N2B	-3.39	117.03	121.78
2	B	2	433	C1D-O1E-C1F	3.35	126.71	121.04
2	B	2	433	C2D-C2E-C2G	3.29	125.37	122.11
2	A	1	433	C1Y-C1D-C1X	-3.20	105.05	110.14
2	A	1	433	O1E-C1F-C1H	3.14	132.30	119.16
2	B	2	433	C3F-C3D-CL3D	3.03	123.92	120.02
2	A	1	433	C2C-N2B-C1N	2.90	123.34	116.69
2	A	1	433	C1H-C1F-C1G	-2.84	115.81	120.18
2	A	1	433	C1J-C1H-C1F	2.77	123.13	119.73
2	A	1	433	C1I-C1G-C1F	2.73	123.08	119.73
2	B	2	433	C3G-C3F-C3D	2.72	123.55	120.58
2	B	2	433	O1E-C1F-C1H	2.68	130.39	119.16
2	B	2	433	C2C-N2B-C1N	2.61	122.68	116.69
2	A	1	433	O2A-C2A-N3A	-2.57	117.93	123.61
2	A	1	433	C2H-C2F-CL2F	-2.52	113.35	118.41
2	B	2	433	C3E-C3C-C3B	2.48	123.78	118.62
2	A	1	433	C3G-C3F-C3D	2.39	123.19	120.58
2	A	1	433	C2E-C2F-CL2F	2.34	124.02	119.60
2	B	2	433	C1H-C1F-C1G	-2.30	116.63	120.18
2	A	1	433	C3E-C3C-C3B	2.21	123.21	118.62
2	B	2	433	C2J-C2H-C2F	2.18	122.69	119.39
2	B	2	433	C3C-C3B-N3A	2.15	126.78	121.80
2	A	1	433	C2J-C2H-C2F	2.14	122.63	119.39

There are no chirality outliers.
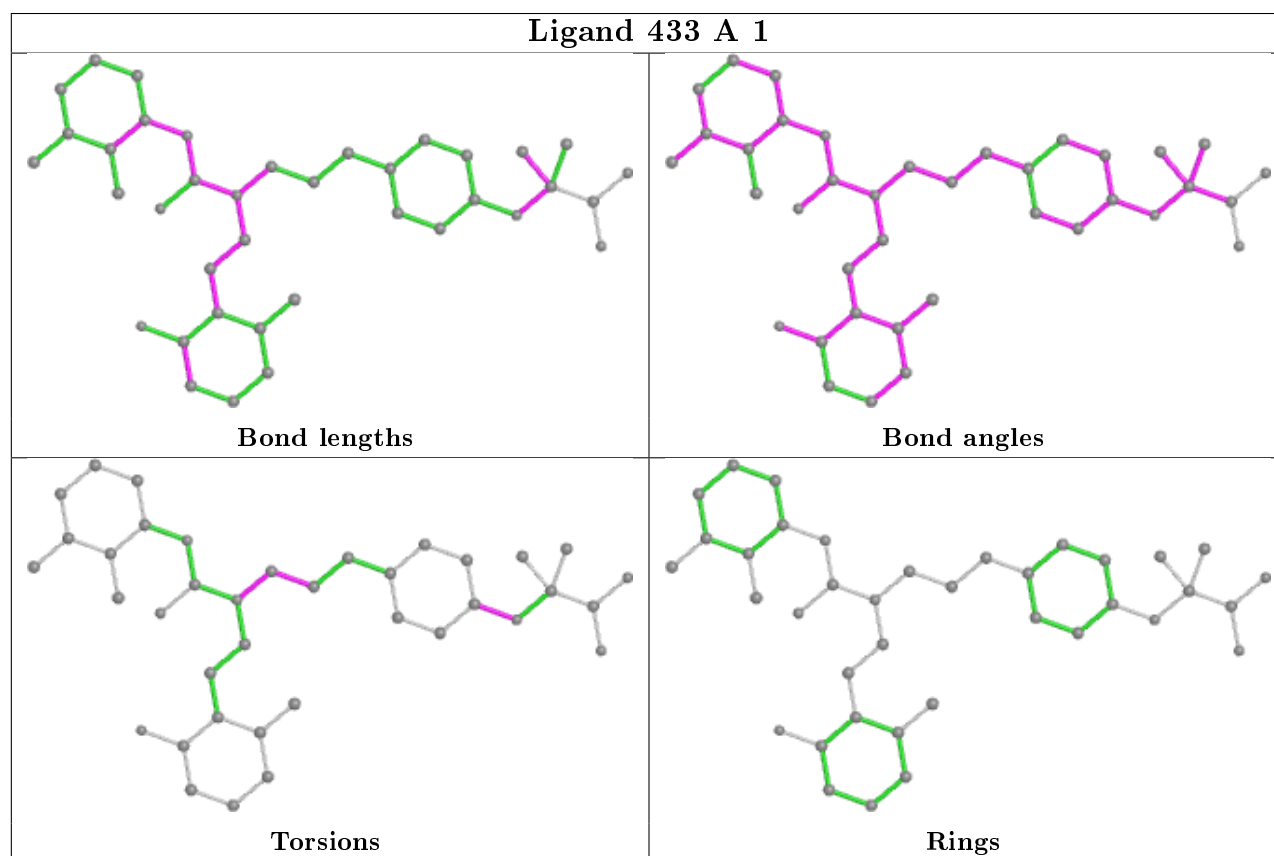
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	433	C1L-C1M-C1N-N2B
2	B	2	433	C1L-C1M-C1N-N2B
2	A	1	433	C1H-C1F-O1E-C1D
2	B	2	433	C1M-C1N-N2B-C2C
2	A	1	433	C1G-C1F-O1E-C1D
2	B	2	433	C1G-C1F-O1E-C1D
2	B	2	433	C1H-C1F-O1E-C1D
2	B	2	433	C1K-C1L-C1M-C1N
2	A	1	433	C1M-C1N-N2B-C2C

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	433	7	0
2	B	2	433	9	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 433 A 1

Bond lengths

Bond angles

Torsions

Rings

Ligand 433 B 2

Bond lengths

Bond angles

Torsions

Rings

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	271/271 (100%)	0.42	24 (8%)	9	9	25, 48, 103, 114	0
1	B	271/271 (100%)	0.55	29 (10%)	6	5	31, 57, 107, 113	0
All	All	542/542 (100%)	0.48	53 (9%)	7	7	25, 52, 105, 114	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	GLY	9.3
1	A	274	TYR	7.3
1	B	241	ALA	7.0
1	A	265	LYS	6.9
1	B	244	THR	6.3
1	B	274	TYR	6.0
1	A	269	ASN	5.8
1	A	207	GLN	5.6
1	B	273	PRO	5.5
1	B	242	SER	5.3
1	A	270	GLY	5.2
1	B	265	LYS	5.1
1	B	209	ALA	4.9
1	A	241	ALA	4.9
1	B	240	LYS	4.9
1	B	263	VAL	4.8
1	A	247	PHE	4.8
1	A	208	VAL	4.8
1	B	268	VAL	4.7
1	B	264	TRP	4.7
1	B	433	PRO	4.4
1	A	240	LYS	4.2
1	B	430	TYR	3.8
1	A	264	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	477	TYR	3.7
1	B	243	HIS	3.6
1	B	272	PRO	3.5
1	B	270	GLY	3.4
1	B	462	GLU	3.3
1	A	212	LYS	3.3
1	A	272	PRO	3.2
1	B	475	ASP	3.2
1	A	430	TYR	3.2
1	A	268	VAL	3.2
1	A	273	PRO	3.1
1	B	208	VAL	3.1
1	B	271	LEU	3.0
1	A	267	LEU	2.9
1	B	260	LYS	2.9
1	B	239	GLY	2.7
1	A	262	LEU	2.7
1	A	271	LEU	2.7
1	B	238	THR	2.7
1	A	243	HIS	2.6
1	B	431	LEU	2.5
1	A	263	VAL	2.5
1	A	477	TYR	2.3
1	B	262	LEU	2.3
1	A	363	ILE	2.2
1	B	358	LYS	2.2
1	A	209	ALA	2.1
1	B	227	ASN	2.1
1	B	427	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.
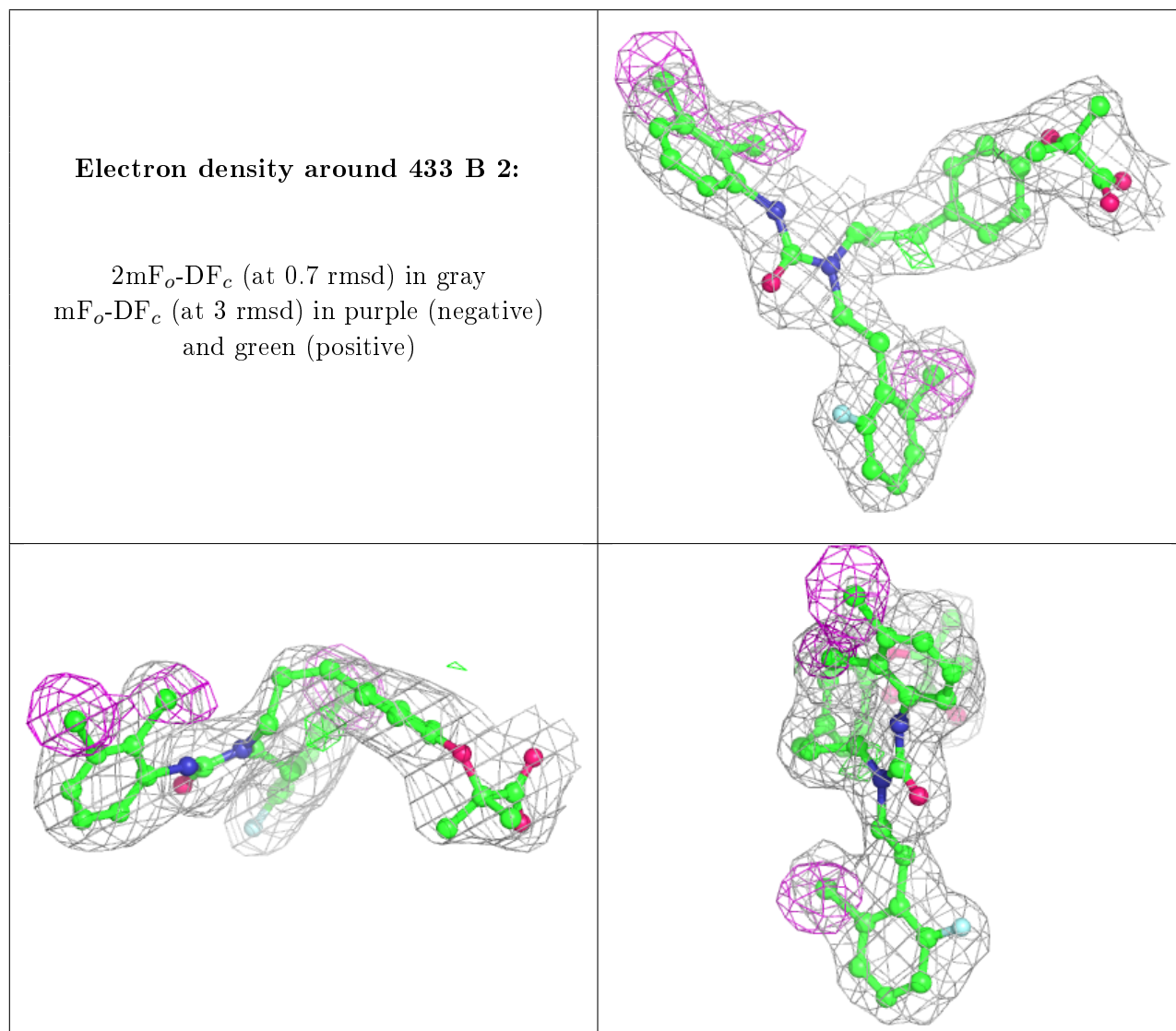
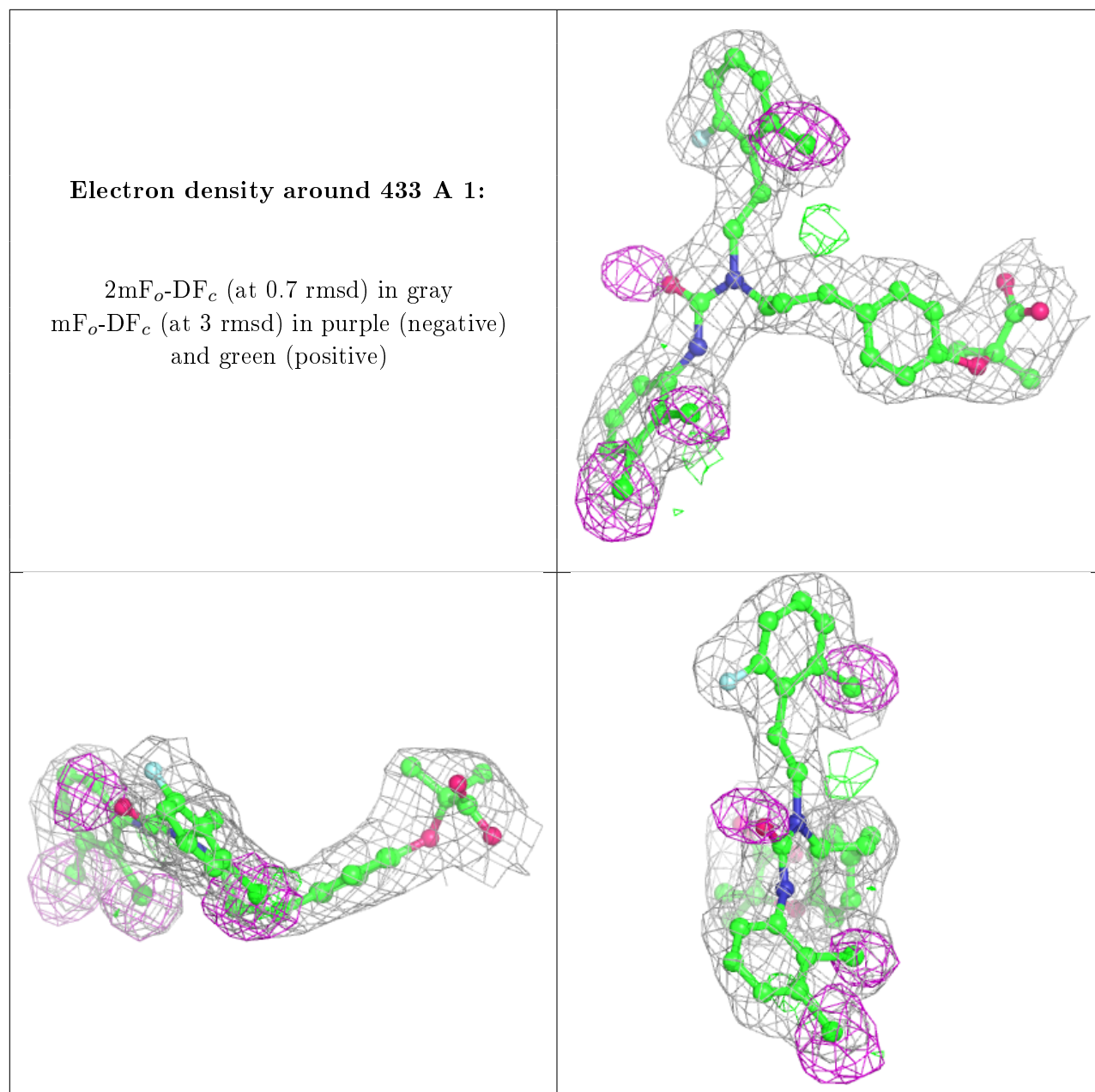## 6.3 Carbohydrates (i)

There are no carbohydrates 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
2	433	B	2	38/38	0.85	0.18	36,45,54,54	0
2	433	A	1	38/38	0.90	0.17	19,35,44,46	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 433 B 2:

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

Electron density around 433 A 1:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.