Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 04:26 PM EDT

PDB ID	:	2GYV
Title	:	Crystal structure of Mus musculus Acetylcholinesterase in complex with Ortho-7
Authors	:	Pang, Y.P.; Boman, M.; Artursson, E.; Akfur, C.; Lundberg, S.
Deposited on	:	2006-05-10
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.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

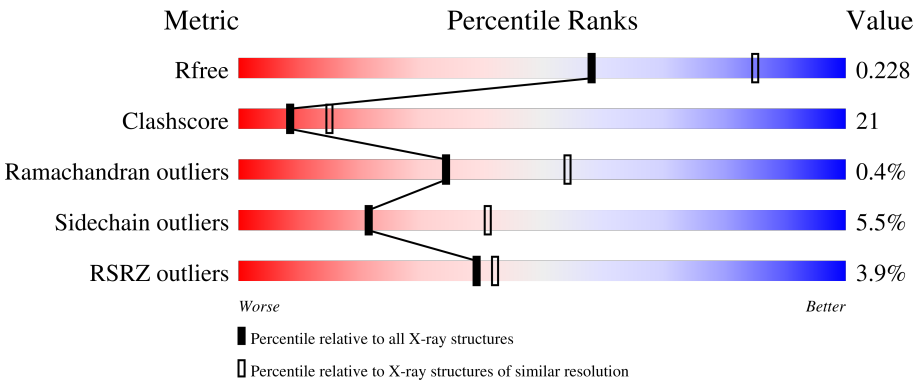
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	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 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	543	5% 56% 41%
1	B	543	3% 62% 34%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1407	-	-	-	X
3	CO3	A	1408	-	-	X	-
3	CO3	B	544	-	-	X	-
4	HBP	A	1409	-	-	X	-
4	HBP	B	545	-	-	X	-

2 Entry composition (i)

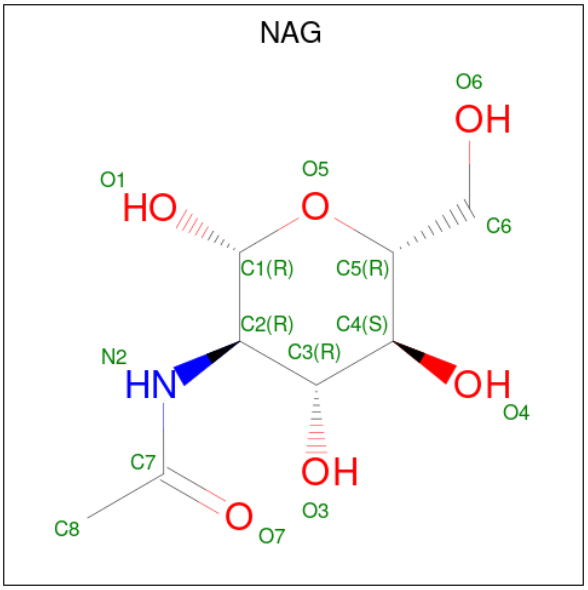
There are 6 unique types of molecules in this entry. The entry contains 8771 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

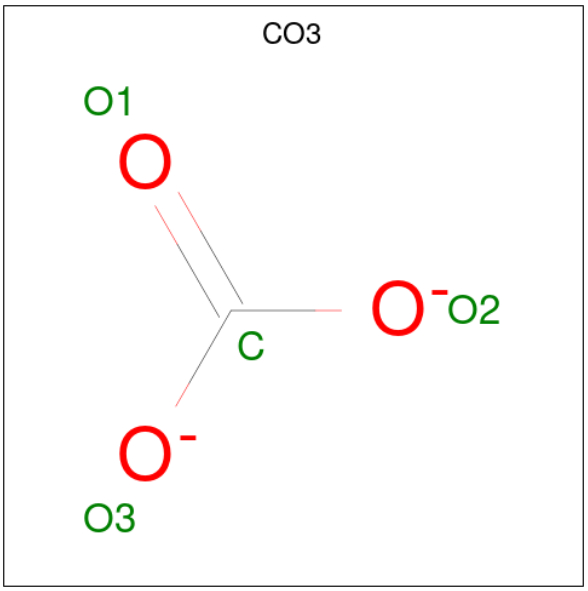
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	535	4177	2679	725	759	14	0	0	0
1	B	533	4159	2670	718	757	14	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



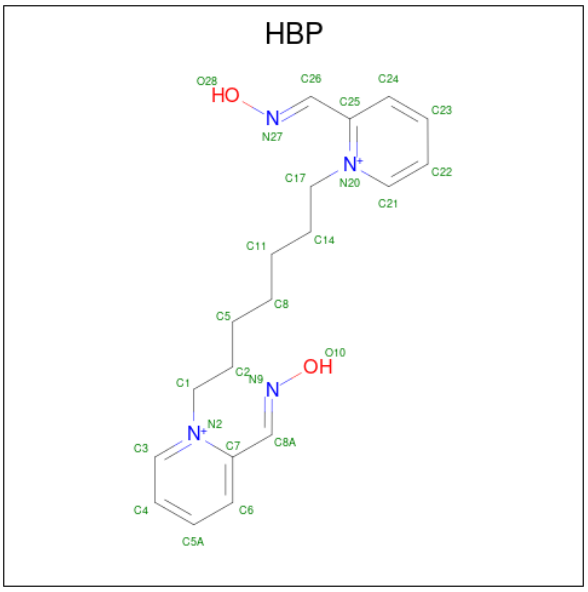
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	13	8	1	4	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 4 is 1,7-HEPTYLENE-BIS-N,N'-SYN-2-PYRIDINIUMALDOXIME (three-letter code: HBP) (formula: $C_{19}H_{26}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	25	19	4	2	0	0

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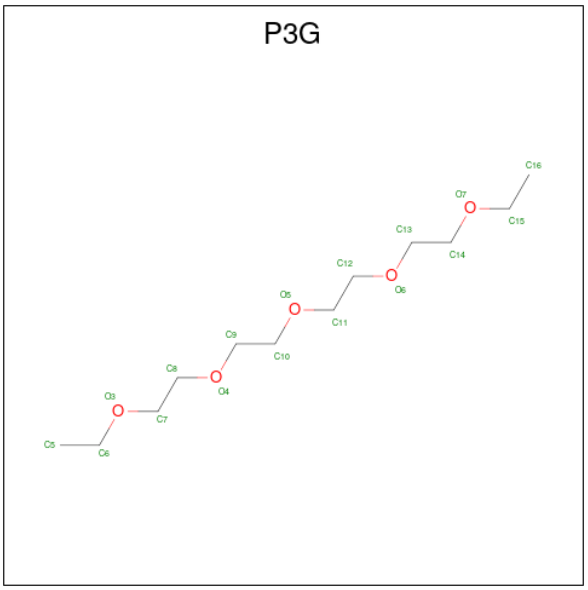
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	25	19	4	2	0	0

- Molecule 5 is 3,6,9,12,15-PENTAOXAHEPTADECANE (three-letter code: P3G) (formula: $C_{12}H_{26}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	7	5	2	0	0

- Molecule 6 is water.

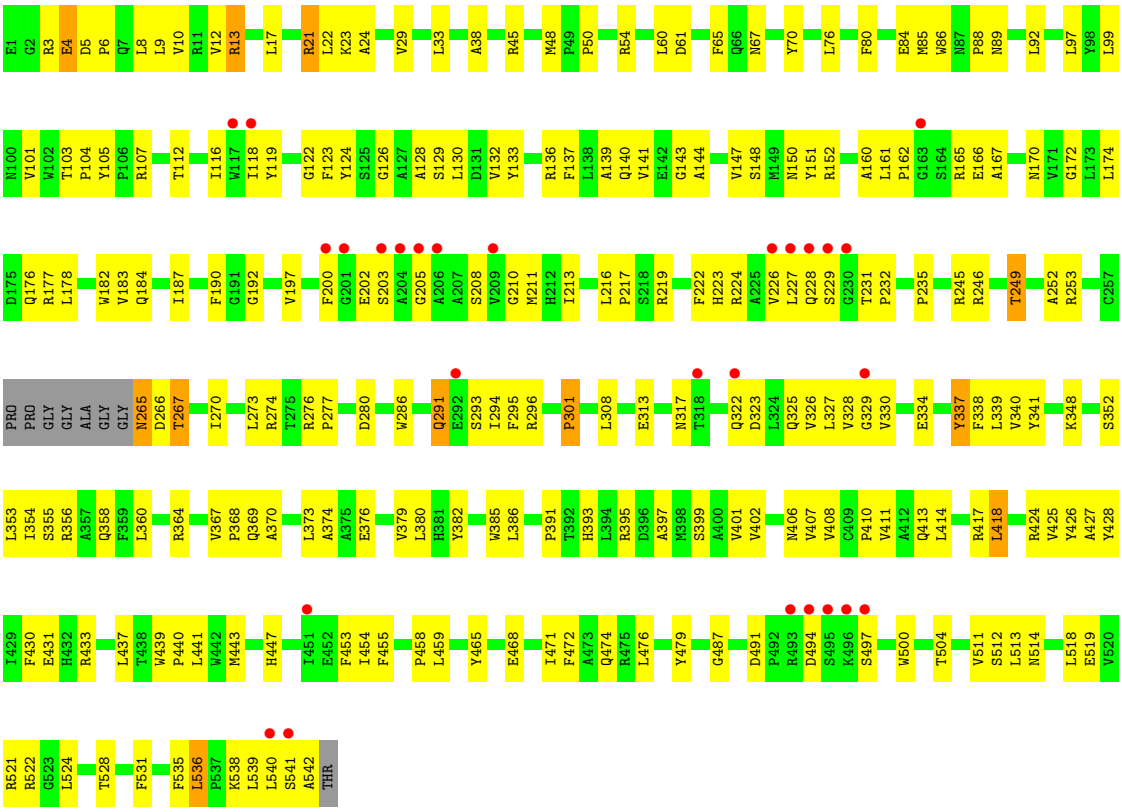
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	194	194	194	0	0
6	B	149	149	149	0	0

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.

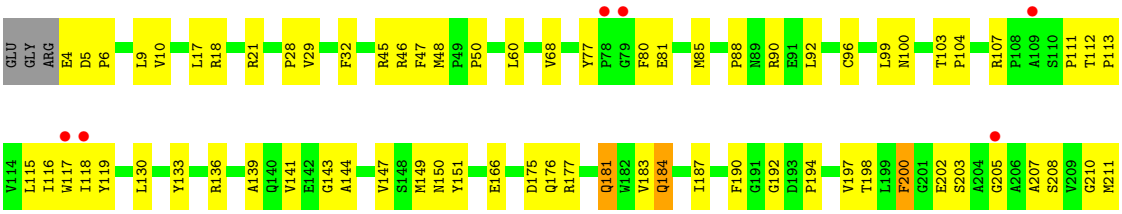
- Molecule 1: Acetylcholinesterase

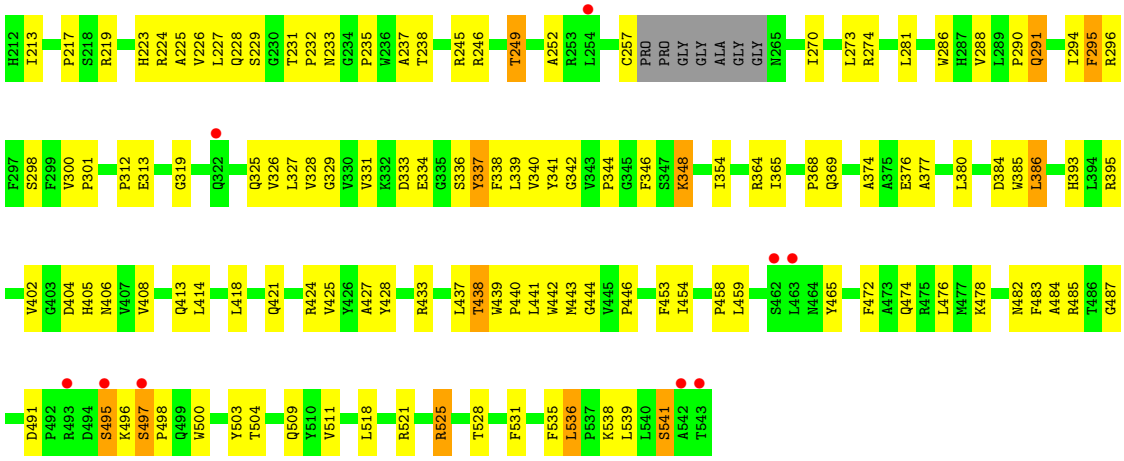
Chain A:



- Molecule 1: Acetylcholinesterase

Chain B:




H212 I213 P217 S218 R219 H223 R224 A225 V226 L227 Q228 S229 G230 T231 P232 N233 G234 P235 W236 A237 T238 R245 R246 T249 A252 R253 L254 C257 PRO PRO GLY GLY ALA GLY GLY N265 I270 L273 R274 L281 W286 H287 V288 L289 P290 Q291 I294 F295 R296
F297 S298 F299 V300 P301 P312 E313 G319 Q322 Q325 V326 L327 V328 G329 V330 V331 K332 D333 E334 G335 S336 Y337 F338 L339 V340 Y341 G342 V343 P344 G345 F346 S347 K348 I354 R364 I365 P368 Q369 A374 A375 E376 A377 L380 D384 W385 L386 H393 L394 R395
V402 G403 D404 H405 N406 V407 V408 Q413 L414 L418 Q421 R424 V425 Y426 A427 Y428 R433 L437 T438 W439 P440 L441 W442 M443 G444 V445 P446 F453 I454 P458 L459 S462 L463 M464 Y465 F472 A473 Q474 R475 L476 M477 K478 N482 F483 A484 R485 T486 G487
D491 P492 R493 D494 S495 K496 S497 P498 Q499 W500 Y503 T504 Q509 Y510 V511 L518 R521 R525 T528 F531 F535 L536 P537 K538 L539 L540 S541 A542 T543

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.73Å 108.58Å 220.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.50 28.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.00-2.50) 99.3 (28.95-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.241 0.188 , 0.228	Depositor DCC
R_{free} test set	1276 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8771	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: CO3, NAG, P3G, HBP

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	0.75	0/4300	0.77	1/5875 (0.0%)
1	B	0.68	0/4282	0.71	0/5851
All	All	0.71	0/8582	0.74	1/11726 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	LEU	CA-CB-CG	-5.63	102.36	115.30

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	4177	0	4063	182	0
1	B	4159	0	4047	155	0
2	A	27	0	26	0	0
3	A	4	0	0	3	0
3	B	4	0	0	2	0
4	A	25	0	26	15	0
4	B	25	0	26	9	0
5	B	7	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	194	0	0	13	0
6	B	149	0	0	11	0
All	All	8771	0	8194	342	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 21.

All (342) 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)
4:A:1409:HBP:H26	4:A:1409:HBP:H16	1.18	1.10
1:B:245:ARG:O	1:B:249:THR:HG23	1.57	1.03
1:B:197:VAL:H	1:B:223:HIS:HD2	1.07	1.00
1:A:203:SER:HG	3:A:1408:CO3:C	1.82	0.93
4:A:1409:HBP:H16	4:A:1409:HBP:C26	2.00	0.92
1:B:197:VAL:H	1:B:223:HIS:CD2	1.89	0.90
4:A:1409:HBP:H26	4:A:1409:HBP:C14	2.03	0.88
1:A:48:MET:HE1	1:A:166:GLU:HA	1.52	0.88
4:B:545:HBP:H1B	4:B:545:HBP:N9	1.90	0.84
1:A:245:ARG:O	1:A:249:THR:HG23	1.78	0.83
1:A:197:VAL:H	1:A:223:HIS:CD2	1.96	0.83
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.62	0.80
1:B:136:ARG:HD2	6:B:686:HOH:O	1.81	0.79
4:B:545:HBP:H16	4:B:545:HBP:H26	1.64	0.79
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.17	0.78
1:A:266:ASP:O	1:A:270:ILE:HD12	1.84	0.78
1:A:197:VAL:H	1:A:223:HIS:HD2	1.30	0.75
1:B:369:GLN:HB2	6:B:562:HOH:O	1.86	0.75
1:A:535:PHE:HB2	1:B:380:LEU:HD12	1.70	0.73
1:A:203:SER:OG	3:A:1408:CO3:O2	2.06	0.73
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.69	0.73
1:B:112:THR:HG21	1:B:143:GLY:O	1.90	0.71
1:B:207:ALA:O	1:B:211:MET:HG2	1.90	0.71
1:B:525:ARG:HH11	1:B:525:ARG:CG	2.02	0.71
1:A:227:LEU:HD22	1:A:414:LEU:HD21	1.71	0.71
1:B:497:SER:H	1:B:498:PRO:HA	1.56	0.70
4:A:1409:HBP:H1B	4:A:1409:HBP:N9	2.07	0.70
1:B:328:VAL:O	1:B:427:ALA:HA	1.91	0.70
1:A:286:TRP:HB2	4:A:1409:HBP:C6	2.22	0.69
1:A:48:MET:HE1	1:A:166:GLU:CA	2.23	0.69
1:A:48:MET:HE1	1:A:165:ARG:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ARG:HH11	1:B:525:ARG:HG2	1.58	0.67
1:A:424:ARG:HD2	6:A:1440:HOH:O	1.96	0.66
1:B:286:TRP:HB2	4:B:545:HBP:C6	2.26	0.65
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.77	0.65
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.32	0.65
4:B:545:HBP:H26	4:B:545:HBP:C14	2.24	0.65
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.31	0.65
1:B:77:TYR:CZ	1:B:348:LYS:HG2	2.32	0.64
1:B:104:PRO:HG3	1:B:143:GLY:HA2	1.79	0.64
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.81	0.63
1:A:176:GLN:OE1	1:A:208:SER:HB3	1.98	0.63
1:B:224:ARG:HD3	1:B:487:GLY:CA	2.29	0.62
4:A:1409:HBP:C26	4:A:1409:HBP:C14	2.68	0.61
1:A:112:THR:HG21	1:A:143:GLY:O	2.00	0.61
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.82	0.61
1:A:337:TYR:HA	1:A:443:MET:CE	2.30	0.61
1:B:88:PRO:HG2	1:B:92:LEU:HD21	1.83	0.61
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.81	0.61
1:A:277:PRO:HG2	1:A:280:ASP:HB2	1.83	0.61
1:A:522:ARG:HB3	1:B:386:LEU:HD21	1.81	0.61
1:B:80:PHE:CE1	1:B:438:THR:HB	2.35	0.61
1:B:231:THR:HB	1:B:233:ASN:OD1	2.01	0.61
1:A:141:VAL:HG21	1:A:459:LEU:HD23	1.83	0.61
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.82	0.61
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.30	0.60
1:A:538:LYS:HE3	1:B:376:GLU:OE2	2.00	0.60
1:B:200:PHE:CB	1:B:226:VAL:HB	2.31	0.60
1:B:496:LYS:HB2	6:B:581:HOH:O	2.01	0.60
1:B:141:VAL:HG21	1:B:459:LEU:CD2	2.32	0.59
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.03	0.59
1:B:203:SER:HG	3:B:544:CO3:C	2.13	0.59
1:B:374:ALA:HA	1:B:539:LEU:HD23	1.85	0.59
1:B:197:VAL:N	1:B:223:HIS:HD2	1.90	0.59
4:A:1409:HBP:N9	4:A:1409:HBP:C1	2.65	0.58
1:A:38:ALA:HB2	1:A:178:LEU:HD23	1.86	0.58
1:A:337:TYR:HA	1:A:443:MET:HE1	1.84	0.58
1:A:328:VAL:O	1:A:427:ALA:HA	2.03	0.58
1:B:184:GLN:OE1	1:B:194:PRO:HB2	2.04	0.58
1:B:274:ARG:HD3	6:B:568:HOH:O	2.04	0.58
4:B:545:HBP:N9	4:B:545:HBP:C1	2.63	0.58
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:NH1	6:A:1547:HOH:O	2.33	0.58
1:B:96:CYS:O	1:B:150:ASN:HB2	2.04	0.58
1:B:459:LEU:HD11	1:B:474:GLN:HG3	1.86	0.58
1:A:374:ALA:HB1	1:A:536:LEU:HD21	1.86	0.58
1:A:235:PRO:HB2	1:A:296:ARG:NH2	2.18	0.57
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.85	0.57
1:B:203:SER:OG	3:B:544:CO3:O1	2.22	0.57
1:A:118:ILE:O	1:A:205:GLY:HA3	2.04	0.57
1:A:424:ARG:CD	6:A:1440:HOH:O	2.53	0.57
1:A:200:PHE:CB	1:A:226:VAL:HB	2.35	0.56
1:A:84:GLU:HG3	6:A:1593:HOH:O	2.03	0.56
1:A:166:GLU:OE2	1:A:267:THR:HG23	2.05	0.56
1:A:337:TYR:CE2	1:A:341:TYR:HE1	2.24	0.56
1:B:245:ARG:O	1:B:249:THR:CG2	2.44	0.56
1:B:341:TYR:CE2	4:B:545:HBP:H12	2.40	0.56
1:A:227:LEU:HD22	1:A:414:LEU:CD2	2.36	0.56
1:B:313:GLU:HG2	6:B:580:HOH:O	2.06	0.56
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.86	0.55
1:B:497:SER:N	1:B:498:PRO:HA	2.19	0.55
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.88	0.55
1:B:10:VAL:HG22	1:B:107:ARG:HH11	1.72	0.55
1:B:326:VAL:HG21	1:B:418:LEU:HD13	1.88	0.55
1:B:197:VAL:N	1:B:223:HIS:CD2	2.70	0.54
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.89	0.54
1:B:504:THR:HB	6:B:602:HOH:O	2.07	0.54
4:B:545:HBP:C14	4:B:545:HBP:C26	2.84	0.54
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.37	0.54
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.90	0.54
1:A:339:LEU:HD11	1:A:399:SER:HA	1.90	0.54
1:A:197:VAL:HB	1:A:222:PHE:HA	1.89	0.54
1:B:252:ALA:HA	1:B:273:LEU:HD21	1.89	0.54
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.88	0.54
1:A:203:SER:CB	3:A:1408:CO3:C	2.80	0.53
1:B:118:ILE:O	1:B:205:GLY:HA3	2.07	0.53
1:A:355:SER:OG	1:A:358:GLN:HG3	2.08	0.53
1:B:81:GLU:HB3	1:B:438:THR:HG21	1.90	0.53
1:B:444:GLY:O	1:B:446:PRO:HD3	2.09	0.53
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.91	0.53
1:A:313:GLU:HG3	6:A:1558:HOH:O	2.08	0.53
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.90	0.53
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.44	0.52
1:A:514:ASN:HB2	6:A:1461:HOH:O	2.09	0.52
1:B:319:GLY:O	1:B:421:GLN:HG3	2.09	0.52
1:B:341:TYR:CZ	4:B:545:HBP:H12	2.45	0.52
1:A:380:LEU:HD12	1:B:535:PHE:HB2	1.92	0.52
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.92	0.52
1:A:139:ALA:HA	1:A:144:ALA:O	2.10	0.52
1:A:430:PHE:HE2	1:A:476:LEU:HD11	1.75	0.52
1:A:380:LEU:HA	1:A:385:TRP:HZ2	1.76	0.52
1:A:337:TYR:HE2	1:A:341:TYR:HE1	1.56	0.51
1:B:404:ASP:HA	1:B:408:VAL:HB	1.92	0.51
1:A:228:GLN:HG2	1:A:428:TYR:OH	2.10	0.51
1:A:337:TYR:CE2	4:A:1409:HBP:C26	2.94	0.51
1:B:295:PHE:CE2	1:B:338:PHE:CE1	2.98	0.51
1:A:128:ALA:HB1	1:A:148:SER:OG	2.10	0.51
1:A:337:TYR:CD2	4:A:1409:HBP:N27	2.78	0.51
1:A:352:SER:O	1:A:395:ARG:HG3	2.11	0.51
1:A:376:GLU:HG2	1:B:538:LYS:HD2	1.93	0.51
1:A:424:ARG:HG2	1:A:426:TYR:CE1	2.46	0.51
1:B:346:PHE:CE1	1:B:354:ILE:HG21	2.46	0.51
1:B:472:PHE:CZ	1:B:476:LEU:HD11	2.46	0.51
1:B:495:SER:OG	1:B:496:LYS:N	2.43	0.51
1:B:374:ALA:HA	1:B:539:LEU:CD2	2.41	0.50
1:A:286:TRP:CE3	4:A:1409:HBP:C3	2.94	0.50
1:A:479:TYR:OH	1:A:518:LEU:HG	2.12	0.50
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.92	0.50
1:B:213:ILE:O	1:B:219:ARG:HD3	2.11	0.50
1:B:393:HIS:HB3	6:B:626:HOH:O	2.10	0.50
1:A:21:ARG:HG3	1:A:105:TYR:CE1	2.47	0.50
1:A:50:PRO:HD2	1:A:174:LEU:HB3	1.94	0.50
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.92	0.50
1:B:227:LEU:HD22	1:B:414:LEU:HD21	1.94	0.50
1:A:76:LEU:HD22	1:A:341:TYR:CD2	2.47	0.50
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.92	0.50
1:A:471:ILE:HA	1:A:474:GLN:HE21	1.77	0.50
1:A:541:SER:O	1:A:542:ALA:HB2	2.10	0.50
1:A:382:TYR:O	1:A:393:HIS:HE1	1.94	0.50
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.94	0.49
1:A:431:GLU:CD	1:A:521:ARG:HH12	2.14	0.49
1:B:46:ARG:HB3	1:B:274:ARG:HG2	1.95	0.49
1:A:337:TYR:CG	4:A:1409:HBP:N27	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG11	1:B:443:MET:CE	2.42	0.49
1:A:86:TRP:CG	4:A:1409:HBP:H22	2.48	0.49
1:A:124:TYR:CD1	1:A:124:TYR:C	2.86	0.49
1:A:137:PHE:HB2	1:A:455:PHE:O	2.13	0.49
1:A:397:ALA:O	1:A:401:VAL:HG23	2.13	0.49
1:B:336:SER:HB2	1:B:443:MET:HA	1.95	0.49
1:A:122:GLY:O	1:A:123:PHE:HB2	2.13	0.49
1:B:337:TYR:HB2	6:B:604:HOH:O	2.13	0.49
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.43	0.48
1:B:525:ARG:CG	1:B:525:ARG:NH1	2.71	0.48
1:B:103:THR:HG21	1:B:190:PHE:HB3	1.94	0.48
1:A:252:ALA:HA	1:A:273:LEU:HD21	1.94	0.48
1:B:181:GLN:HG2	6:B:673:HOH:O	2.13	0.48
1:B:380:LEU:HD22	1:B:385:TRP:CZ2	2.49	0.48
1:A:86:TRP:CB	4:A:1409:HBP:H22	2.44	0.48
1:A:354:ILE:O	1:A:391:PRO:HB3	2.14	0.48
1:A:433:ARG:NH2	1:A:439:TRP:O	2.47	0.48
1:B:376:GLU:O	1:B:380:LEU:HG	2.13	0.48
1:B:478:LYS:HD2	1:B:491:ASP:OD2	2.14	0.48
1:B:119:TYR:CE1	1:B:151:TYR:CE1	3.02	0.47
1:B:141:VAL:HG21	1:B:459:LEU:HD23	1.96	0.47
1:A:50:PRO:HB2	1:A:178:LEU:HD22	1.95	0.47
1:A:376:GLU:O	1:A:380:LEU:HG	2.14	0.47
1:B:348:LYS:HA	1:B:440:PRO:HG3	1.96	0.47
1:A:167:ALA:HB2	1:A:270:ILE:HG12	1.96	0.47
1:A:213:ILE:HA	1:A:219:ARG:HD3	1.95	0.47
1:A:231:THR:HG21	1:A:411:VAL:HA	1.97	0.47
1:B:340:VAL:HG11	1:B:443:MET:HE1	1.96	0.47
1:A:5:ASP:C	1:A:5:ASP:OD1	2.53	0.47
1:A:293:SER:HB3	1:A:368:PRO:HB3	1.97	0.47
1:A:360:LEU:CD2	1:A:379:VAL:HG11	2.44	0.47
1:B:107:ARG:HB3	6:B:583:HOH:O	2.14	0.47
1:B:224:ARG:HD2	1:B:483:PHE:O	2.15	0.47
1:B:238:THR:HA	1:B:301:PRO:O	2.14	0.47
1:A:338:PHE:HZ	1:A:447:HIS:CD2	2.33	0.47
1:A:374:ALA:HA	1:A:539:LEU:HD23	1.97	0.47
1:A:183:VAL:HG13	1:A:187:ILE:HB	1.97	0.47
1:B:425:VAL:O	1:B:503:TYR:N	2.43	0.46
1:B:46:ARG:HD3	1:B:47:PHE:CZ	2.51	0.46
1:B:327:LEU:HD11	1:B:500:TRP:CH2	2.49	0.46
1:A:224:ARG:CD	1:A:487:GLY:HA2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:HB2	6:A:1435:HOH:O	2.16	0.46
1:A:504:THR:HB	6:A:1585:HOH:O	2.16	0.46
1:B:296:ARG:HG2	6:B:641:HOH:O	2.15	0.46
1:A:468:GLU:CD	1:A:468:GLU:H	2.18	0.46
1:B:337:TYR:HD2	1:B:337:TYR:O	1.99	0.46
1:A:338:PHE:CZ	1:A:447:HIS:CD2	3.04	0.46
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.50	0.46
1:B:213:ILE:HD11	1:B:225:ALA:CB	2.46	0.46
1:A:224:ARG:HD3	1:A:487:GLY:HA2	1.98	0.46
1:A:330:VAL:HG11	1:A:408:VAL:HA	1.98	0.46
1:B:100:ASN:O	1:B:147:VAL:HA	2.16	0.46
1:A:428:TYR:HB3	1:A:500:TRP:CZ2	2.51	0.46
1:B:528:THR:O	1:B:531:PHE:HB3	2.16	0.46
1:B:116:ILE:HD11	1:B:183:VAL:HG11	1.98	0.45
1:B:210:GLY:CA	1:B:232:PRO:HG3	2.45	0.45
1:B:509:GLN:HA	1:B:521:ARG:O	2.16	0.45
1:A:337:TYR:HA	1:A:443:MET:HE3	1.98	0.45
1:B:536:LEU:HD22	1:B:536:LEU:HA	1.87	0.45
1:B:187:ILE:HD12	1:B:187:ILE:HA	1.83	0.45
1:B:227:LEU:HD22	1:B:414:LEU:CD2	2.47	0.45
1:A:22:LEU:HD13	1:A:136:ARG:NH1	2.32	0.45
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.99	0.45
1:A:101:VAL:HG22	1:A:147:VAL:HG22	1.98	0.45
1:A:119:TYR:CD1	1:A:126:GLY:HA3	2.52	0.45
1:A:317:ASN:OD1	1:A:417:ARG:HG3	2.17	0.45
1:B:202:GLU:HA	1:B:228:GLN:O	2.17	0.45
1:B:337:TYR:O	1:B:340:VAL:HG22	2.17	0.45
1:A:177:ARG:NH1	1:A:217:PRO:HB2	2.32	0.45
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.99	0.45
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.52	0.45
1:A:334:GLU:CD	1:A:407:VAL:HG11	2.37	0.45
1:A:337:TYR:HE2	1:A:341:TYR:CE1	2.34	0.45
1:A:339:LEU:HD11	1:A:399:SER:CA	2.47	0.45
1:A:291:GLN:HE22	1:A:369:GLN:HE21	1.64	0.44
1:A:326:VAL:O	1:A:425:VAL:HA	2.17	0.44
1:A:364:ARG:N	1:A:364:ARG:HD2	2.32	0.44
1:B:325:GLN:HG3	1:B:424:ARG:HB3	1.98	0.44
1:A:33:LEU:HD22	1:A:65:PHE:CE1	2.53	0.44
1:A:48:MET:HA	1:A:48:MET:CE	2.47	0.44
1:A:337:TYR:CD2	4:A:1409:HBP:C26	3.01	0.44
1:B:210:GLY:HA3	1:B:232:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ILE:HG12	1:B:365:ILE:HG22	2.00	0.44
1:A:86:TRP:HB3	4:A:1409:HBP:H22	1.98	0.44
1:A:160:ALA:O	1:A:162:PRO:HD3	2.18	0.44
1:B:48:MET:SD	1:B:166:GLU:HA	2.58	0.44
1:A:17:LEU:HD23	1:A:60:LEU:HB3	1.99	0.44
1:B:300:VAL:HB	1:B:301:PRO:HD2	2.00	0.44
1:B:511:VAL:CB	1:B:518:LEU:HD22	2.47	0.44
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.17	0.44
1:A:274:ARG:HD3	6:A:1411:HOH:O	2.16	0.44
1:B:291:GLN:HE22	1:B:369:GLN:HE21	1.66	0.44
1:B:340:VAL:CG1	1:B:443:MET:CE	2.96	0.44
1:A:187:ILE:HG13	1:A:192:GLY:HA3	2.00	0.44
1:A:440:PRO:HD2	1:A:443:MET:SD	2.58	0.44
1:B:364:ARG:O	1:B:368:PRO:HA	2.18	0.44
1:B:454:ILE:HD13	1:B:476:LEU:HB3	2.00	0.44
1:A:67:ASN:O	1:A:150:ASN:ND2	2.51	0.44
1:A:85:MET:CE	1:A:132:VAL:HG11	2.48	0.44
1:A:89:ASN:ND2	1:A:129:SER:O	2.41	0.44
1:B:117:TRP:HA	1:B:200:PHE:O	2.17	0.44
1:B:331:VAL:HG22	1:B:334:GLU:OE2	2.17	0.44
1:A:476:LEU:HD22	1:A:513:LEU:HD13	2.00	0.43
1:B:337:TYR:HB3	4:B:545:HBP:O28	2.17	0.43
1:A:61:ASP:OD1	1:A:61:ASP:C	2.57	0.43
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.53	0.43
1:A:512:SER:HB3	1:A:521:ARG:CZ	2.48	0.43
1:B:237:ALA:O	1:B:301:PRO:HD2	2.18	0.43
1:A:10:VAL:HG23	1:A:107:ARG:NH1	2.33	0.43
1:A:5:ASP:OD2	1:A:105:TYR:OH	2.27	0.43
1:B:346:PHE:HE2	1:B:395:ARG:HG2	1.84	0.43
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.53	0.43
1:A:48:MET:CE	1:A:165:ARG:O	2.62	0.43
1:A:202:GLU:HA	1:A:228:GLN:O	2.19	0.43
1:A:172:GLY:O	1:A:176:GLN:HG3	2.19	0.43
1:B:99:LEU:HA	1:B:149:MET:HA	2.00	0.43
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.48	0.43
1:A:48:MET:CE	1:A:166:GLU:HA	2.35	0.43
1:A:152:ARG:HG2	6:A:1416:HOH:O	2.18	0.43
1:A:294:ILE:HD11	1:A:402:VAL:HG21	1.99	0.43
1:A:329:GLY:HA3	1:A:428:TYR:CD2	2.54	0.43
1:A:373:LEU:CD2	1:A:539:LEU:HD11	2.48	0.43
1:A:441:LEU:HD23	1:A:441:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASP:HB3	1:A:8:LEU:HD12	1.99	0.43
1:A:360:LEU:HD12	6:A:1514:HOH:O	2.18	0.43
1:B:4:GLU:OE2	1:B:18:ARG:NH1	2.51	0.42
1:B:139:ALA:HA	1:B:144:ALA:O	2.19	0.42
1:B:333:ASP:OD1	1:B:444:GLY:HA3	2.19	0.42
1:B:380:LEU:HD22	1:B:385:TRP:HZ2	1.84	0.42
1:A:535:PHE:CE1	1:B:377:ALA:HB2	2.54	0.42
1:A:210:GLY:HA3	1:A:232:PRO:HD3	2.01	0.42
1:A:224:ARG:HD3	1:A:487:GLY:CA	2.49	0.42
1:B:433:ARG:NH2	1:B:439:TRP:O	2.44	0.42
1:A:13:ARG:NH2	6:A:1490:HOH:O	2.48	0.42
1:A:216:LEU:HB3	1:A:217:PRO:HD3	2.00	0.42
1:A:227:LEU:N	1:A:227:LEU:HD12	2.34	0.42
1:B:211:MET:HE2	1:B:232:PRO:HA	2.02	0.42
1:A:528:THR:O	1:A:531:PHE:HB3	2.20	0.42
1:B:203:SER:HA	1:B:229:SER:O	2.20	0.42
1:B:235:PRO:HG3	1:B:405:HIS:CE1	2.55	0.42
1:B:290:PRO:HG2	1:B:291:GLN:NE2	2.35	0.42
1:B:294:ILE:HD11	1:B:402:VAL:HG21	2.02	0.42
1:B:440:PRO:HG2	1:B:443:MET:HG3	2.00	0.42
1:B:5:ASP:HA	1:B:6:PRO:HD2	1.94	0.42
1:B:81:GLU:O	1:B:85:MET:HG2	2.20	0.42
1:A:128:ALA:HB1	1:A:148:SER:CB	2.50	0.41
1:A:265:ASN:C	1:A:265:ASN:OD1	2.59	0.41
1:B:50:PRO:HG3	1:B:175:ASP:HA	2.02	0.41
1:B:187:ILE:HG13	1:B:192:GLY:HA3	2.02	0.41
1:B:198:THR:OG1	1:B:484:ALA:HA	2.20	0.41
1:B:346:PHE:CZ	1:B:354:ILE:HD13	2.56	0.41
1:B:478:LYS:O	1:B:482:ASN:HB2	2.20	0.41
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.54	0.41
1:B:252:ALA:HB1	1:B:257:CYS:HB2	2.03	0.41
1:A:80:PHE:CG	1:A:348:LYS:HE2	2.54	0.41
1:A:116:ILE:HA	1:A:147:VAL:O	2.20	0.41
1:A:119:TYR:CE1	1:A:151:TYR:CE1	3.07	0.41
1:A:226:VAL:HA	1:A:327:LEU:O	2.21	0.41
1:A:519:GLU:HB2	6:A:1551:HOH:O	2.20	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.56	0.41
1:A:4:GLU:HG2	1:A:9:LEU:HD21	2.02	0.41
1:A:454:ILE:N	1:A:454:ILE:HD13	2.35	0.41
1:B:384:ASP:HA	5:B:546:P3G:H72	2.03	0.41
1:A:5:ASP:HA	1:A:6:PRO:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:O	1:B:344:PRO:HD3	2.20	0.41
1:A:88:PRO:CG	1:A:92:LEU:HD21	2.51	0.41
1:A:276:ARG:HD3	1:A:276:ARG:HA	1.84	0.41
1:A:337:TYR:O	1:A:340:VAL:HG22	2.21	0.41
1:A:406:ASN:C	1:A:410:PRO:HG2	2.41	0.41
1:A:512:SER:OG	1:A:519:GLU:HB3	2.20	0.41
1:B:9:LEU:HD23	1:B:9:LEU:HA	1.93	0.41
1:A:38:ALA:HB3	1:A:97:LEU:HB3	2.02	0.41
1:A:459:LEU:HD11	1:A:474:GLN:HG3	2.03	0.40
1:B:17:LEU:HD23	1:B:60:LEU:HB3	2.02	0.40
1:B:21:ARG:NH1	1:B:28:PRO:HB3	2.36	0.40
1:B:32:PHE:CG	1:B:190:PHE:HE2	2.39	0.40
1:A:12:VAL:HG11	1:A:182:TRP:CZ2	2.56	0.40
1:A:203:SER:HA	1:A:229:SER:O	2.21	0.40
1:B:211:MET:CE	1:B:301:PRO:HG2	2.52	0.40
1:B:227:LEU:N	1:B:227:LEU:HD12	2.36	0.40
1:B:233:ASN:HA	1:B:312:PRO:HB2	2.03	0.40
1:B:288:VAL:CG2	1:B:298:SER:HB3	2.51	0.40
1:A:491:ASP:HB3	1:A:494:ASP:HB3	2.03	0.40
1:A:10:VAL:CG2	1:A:107:ARG:NH1	2.84	0.40
1:A:99:LEU:HD12	1:A:99:LEU:C	2.41	0.40
1:A:354:ILE:HB	1:A:358:GLN:HB2	2.04	0.40
1:A:367:VAL:HG12	1:A:370:ALA:HB2	2.01	0.40
1:A:430:PHE:HA	1:A:513:LEU:HB2	2.02	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	531/543 (98%)	510 (96%)	21 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	529/543 (97%)	501 (95%)	24 (4%)	4 (1%)	19	35
All	All	1060/1086 (98%)	1011 (95%)	45 (4%)	4 (0%)	34	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	SER
1	B	541	SER
1	B	111	PRO
1	B	497	SER

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	439/443 (99%)	411 (94%)	28 (6%)	17	33
1	B	438/443 (99%)	418 (95%)	20 (5%)	27	50
All	All	877/886 (99%)	829 (94%)	48 (6%)	21	41

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	13	ARG
1	A	21	ARG
1	A	23	LYS
1	A	45	ARG
1	A	54	ARG
1	A	70	TYR
1	A	184	GLN
1	A	246	ARG
1	A	249	THR
1	A	265	ASN

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Mol	Chain	Res	Type
1	A	267	THR
1	A	291	GLN
1	A	295	PHE
1	A	301	PRO
1	A	322	GLN
1	A	323	ASP
1	A	337	TYR
1	A	356	ARG
1	A	386	LEU
1	A	413	GLN
1	A	418	LEU
1	A	437	LEU
1	A	497	SER
1	A	524	LEU
1	A	536	LEU
1	A	540	LEU
1	B	45	ARG
1	B	115	LEU
1	B	181	GLN
1	B	184	GLN
1	B	200	PHE
1	B	246	ARG
1	B	249	THR
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	337	TYR
1	B	348	LYS
1	B	386	LEU
1	B	413	GLN
1	B	437	LEU
1	B	438	THR
1	B	441	LEU
1	B	525	ARG
1	B	536	LEU
1	B	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	223	HIS

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Mol	Chain	Res	Type
1	A	291	GLN
1	A	322	GLN
1	A	393	HIS
1	A	474	GLN
1	B	223	HIS
1	B	287	HIS
1	B	291	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	HBP	B	545	-	26,26,26	0.87	1 (3%)	25,31,31	1.84	4 (16%)
4	HBP	A	1409	-	26,26,26	0.76	1 (3%)	25,31,31	1.69	4 (16%)
3	CO3	B	544	1	2,3,3	0.30	0	2,3,3	0.12	0
2	NAG	A	1407	1	13,13,15	0.97	1 (7%)	16,17,21	2.68	5 (31%)
2	NAG	A	1402	1	14,14,15	0.95	1 (7%)	17,19,21	1.49	3 (17%)
3	CO3	A	1408	1	2,3,3	0.33	0	2,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	P3G	B	546	-	6,6,16	0.55	0	5,5,15	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HBP	B	545	-	-	7/16/16/16	0/2/2/2
4	HBP	A	1409	-	-	8/16/16/16	0/2/2/2
2	NAG	A	1407	1	-	4/5/22/26	0/1/1/1
2	NAG	A	1402	1	-	4/6/23/26	0/1/1/1
5	P3G	B	546	-	-	1/4/4/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	545	HBP	C25-N20	-3.19	1.34	1.37
2	A	1402	NAG	C1-C2	2.47	1.56	1.52
4	A	1409	HBP	C25-N20	-2.26	1.35	1.37
2	A	1407	NAG	C1-C2	2.24	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1407	NAG	C1-O5-C5	7.74	122.68	112.19
4	B	545	HBP	O10-N9-C8A	6.37	123.12	111.86
4	A	1409	HBP	O10-N9-C8A	4.91	120.54	111.86
2	A	1407	NAG	C7-N2-C2	4.72	121.50	114.57
4	A	1409	HBP	C24-C25-N20	4.15	122.61	117.52
4	B	545	HBP	C24-C25-N20	4.10	122.55	117.52
2	A	1402	NAG	C4-C3-C2	3.09	115.55	111.02
2	A	1402	NAG	O5-C5-C6	3.04	111.97	107.20
4	B	545	HBP	C25-C26-N27	2.72	123.01	117.75
2	A	1407	NAG	O3-C3-C4	-2.50	104.56	110.35
2	A	1407	NAG	C4-C3-C2	2.18	114.21	111.02
2	A	1407	NAG	O3-C3-C2	2.15	113.92	109.47
4	A	1409	HBP	C6-C7-N2	2.11	120.11	117.52
2	A	1402	NAG	C2-N2-C7	2.10	125.90	122.90
4	A	1409	HBP	C22-C23-C24	-2.08	117.02	120.19
4	B	545	HBP	C22-C23-C24	-2.05	117.07	120.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1402	NAG	C3-C2-N2-C7
4	A	1409	HBP	C2-C1-N2-C7
4	A	1409	HBP	C2-C1-N2-C3
4	A	1409	HBP	N2-C7-C8A-N9
4	A	1409	HBP	C14-C17-N20-C21
4	A	1409	HBP	C14-C17-N20-C25
4	A	1409	HBP	N2-C1-C2-C5
2	A	1407	NAG	O5-C5-C6-O6
2	A	1407	NAG	C4-C5-C6-O6
5	B	546	P3G	O3-C7-C8-O4
4	B	545	HBP	C11-C14-C17-N20
2	A	1407	NAG	C3-C2-N2-C7
4	B	545	HBP	C1-C2-C5-C8
4	B	545	HBP	C2-C5-C8-C11
2	A	1402	NAG	C1-C2-N2-C7
2	A	1402	NAG	C8-C7-N2-C2
2	A	1407	NAG	C1-C2-N2-C7
4	B	545	HBP	C14-C17-N20-C25
4	B	545	HBP	C6-C7-C8A-N9
2	A	1402	NAG	O7-C7-N2-C2
4	B	545	HBP	C14-C17-N20-C21
4	A	1409	HBP	C2-C5-C8-C11
4	A	1409	HBP	C8-C11-C14-C17
4	B	545	HBP	N2-C7-C8A-N9

There are no ring outliers.

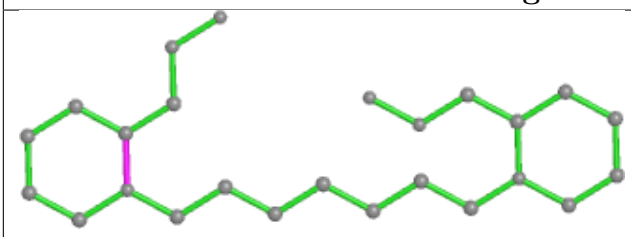
5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	545	HBP	9	0
4	A	1409	HBP	15	0
3	B	544	CO3	2	0
3	A	1408	CO3	3	0
5	B	546	P3G	1	0

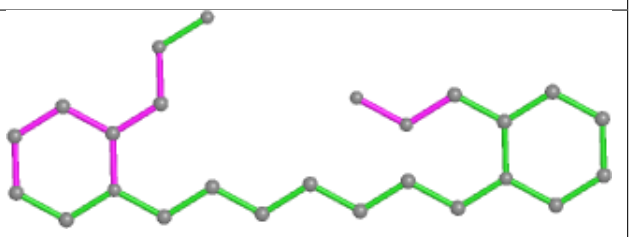
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

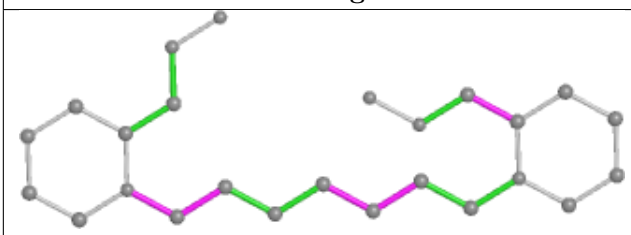
Ligand HBP B 545



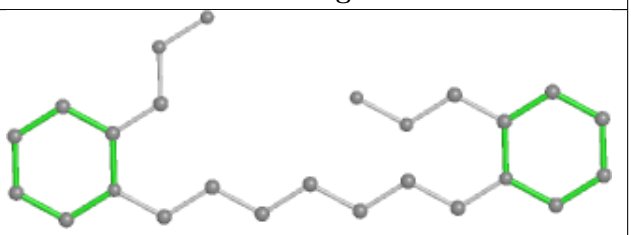
Bond lengths



Bond angles

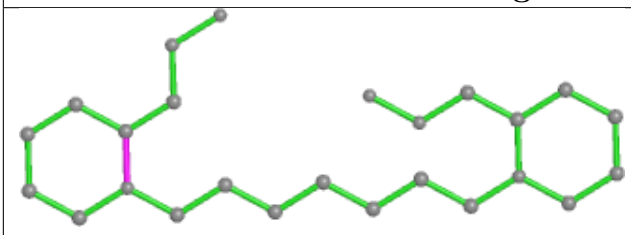


Torsions

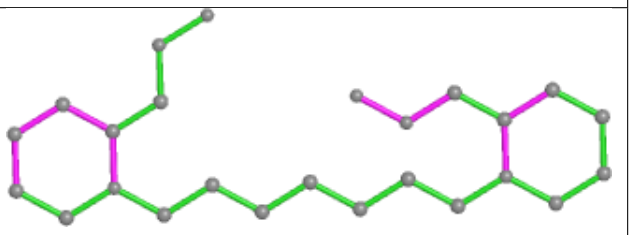


Rings

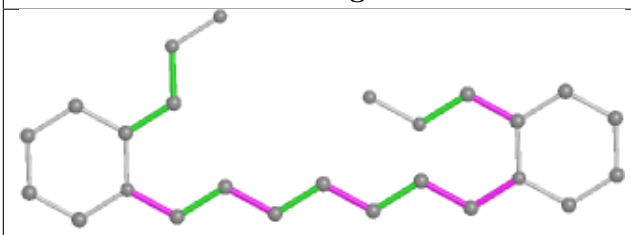
Ligand HBP A 1409



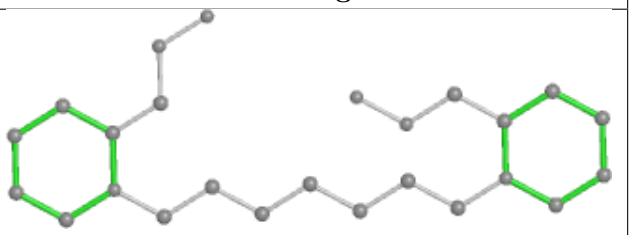
Bond lengths



Bond angles

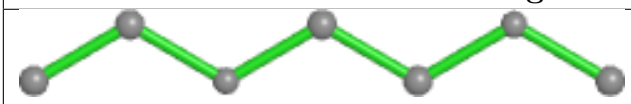


Torsions

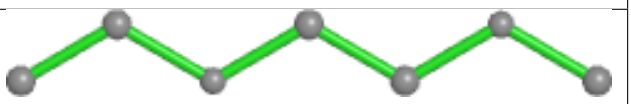


Rings

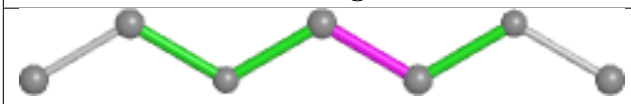
Ligand P3G B 546



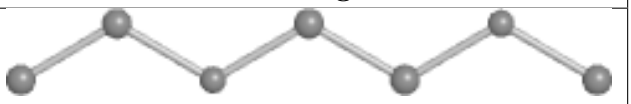
Bond lengths



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	535/543 (98%)	0.05	27 (5%)	28	30	29, 39, 55, 71	0
1	B	533/543 (98%)	0.15	15 (2%)	53	56	32, 40, 53, 74	0
All	All	1068/1086 (98%)	0.10	42 (3%)	39	42	29, 39, 54, 74	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	ARG	4.6
1	B	543	THR	4.2
1	A	495	SER	4.2
1	A	497	SER	4.0
1	B	497	SER	4.0
1	A	494	ASP	3.6
1	A	201	GLY	3.3
1	A	226	VAL	2.9
1	B	109	ALA	2.8
1	A	322	GLN	2.8
1	A	163	GLY	2.8
1	A	206	ALA	2.8
1	A	318	THR	2.8
1	A	541	SER	2.7
1	B	117	TRP	2.7
1	A	118	ILE	2.6
1	A	204	ALA	2.5
1	A	117	TRP	2.5
1	A	200	PHE	2.5
1	A	496	LYS	2.5
1	B	254	LEU	2.5
1	A	228	GLN	2.4
1	A	230	GLY	2.4
1	A	227	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	2.4
1	B	118	ILE	2.4
1	A	451	ILE	2.3
1	A	540	LEU	2.3
1	B	322	GLN	2.3
1	B	78	PRO	2.2
1	A	203	SER	2.2
1	B	542	ALA	2.2
1	B	79	GLY	2.2
1	B	462	SER	2.1
1	A	205	GLY	2.1
1	A	229	SER	2.1
1	B	495	SER	2.1
1	A	292	GLU	2.1
1	B	205	GLY	2.0
1	B	493	ARG	2.0
1	A	209	VAL	2.0
1	B	463	LEU	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
4	HBP	B	545	25/25	0.78	0.35	61,67,78,79	25
2	NAG	A	1407	13/15	0.80	0.40	64,68,69,69	0
4	HBP	A	1409	25/25	0.81	0.26	53,55,56,59	25
2	NAG	A	1402	14/15	0.82	0.52	74,82,82,84	0
5	P3G	B	546	7/17	0.85	0.16	78,80,85,86	0

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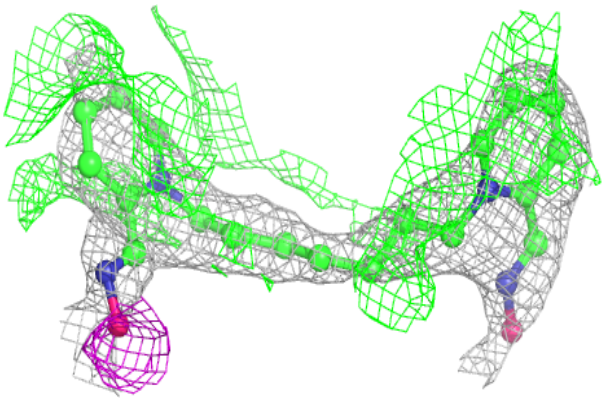
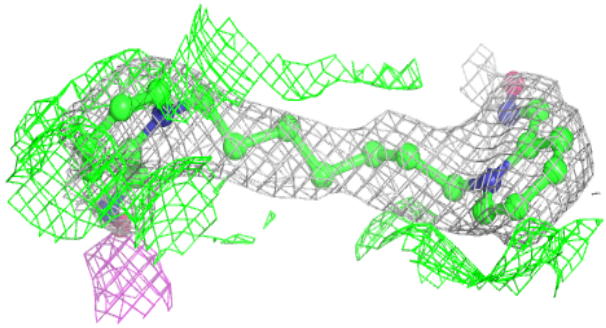
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CO3	A	1408	4/4	0.97	0.16	36,37,37,37	0
3	CO3	B	544	4/4	0.98	0.12	42,42,42,42	0

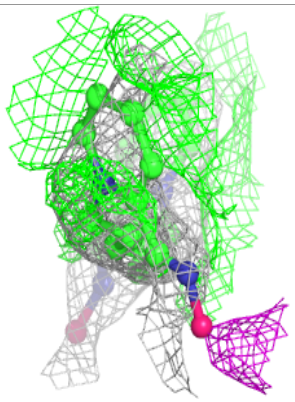
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HBP B 545:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

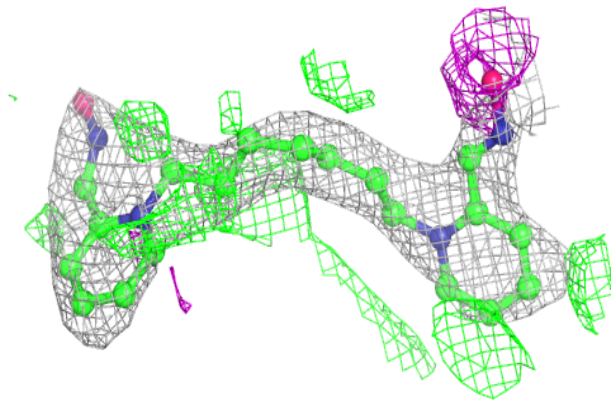


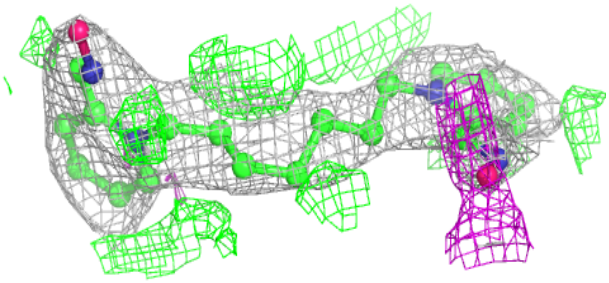


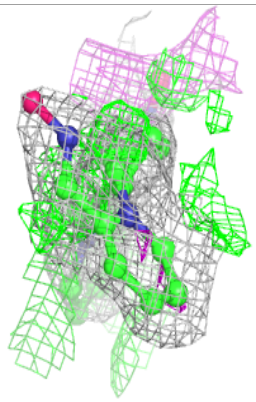


Electron density around HBP A 1409:

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

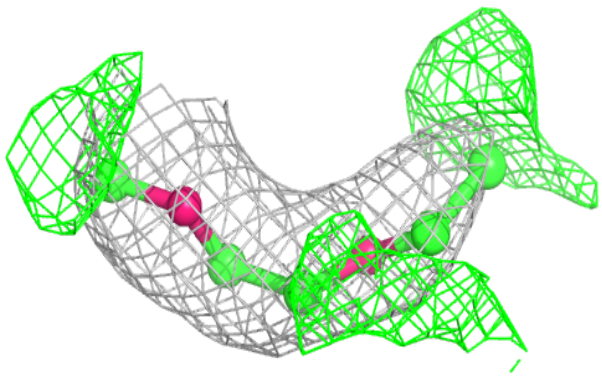


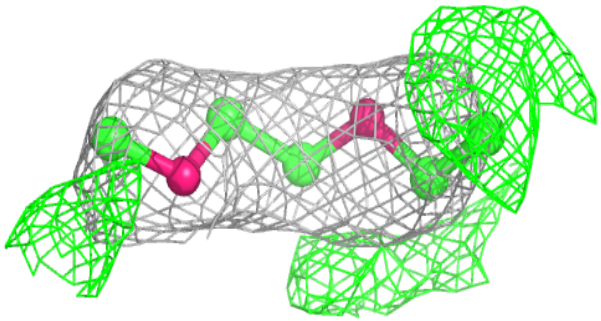


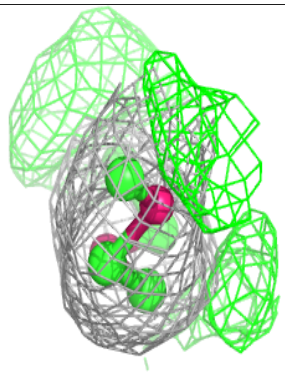


Electron density around P3G B 546:

$2mF_o$-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.