Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 11:00 pm GMT

PDB ID	:	2JEY
Title	:	Mus musculus acetylcholinesterase in complex with HLo-7
Authors	:	Ekstrom, F.; Astot, C.; Pang, Y.P.
Deposited on	:	2007-01-25
Resolution	:	2.70 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:

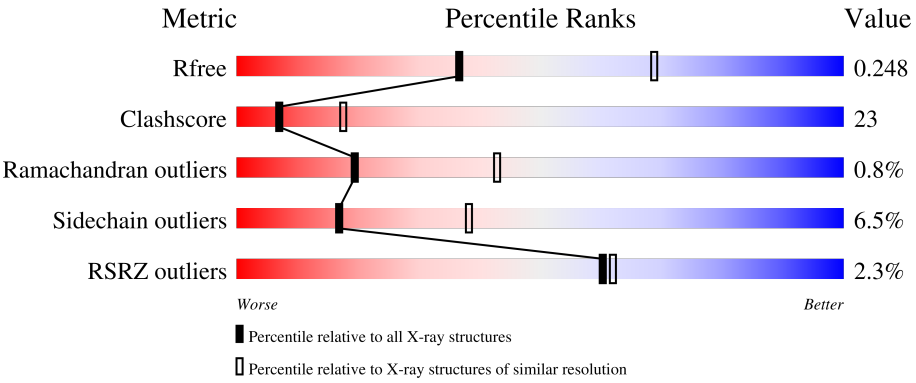
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	548	2% 53% 42%
1	B	548	3% 54% 39%

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
3	P6G	B	1546	-	X	-	-

2 Entry composition

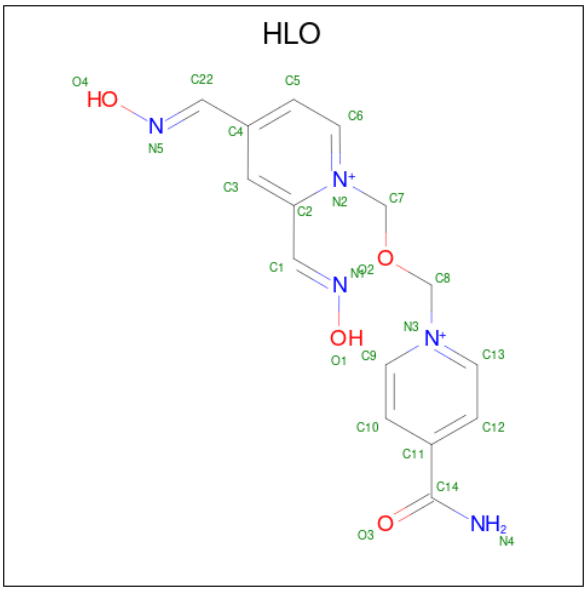
There are 4 unique types of molecules in this entry. The entry contains 8565 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

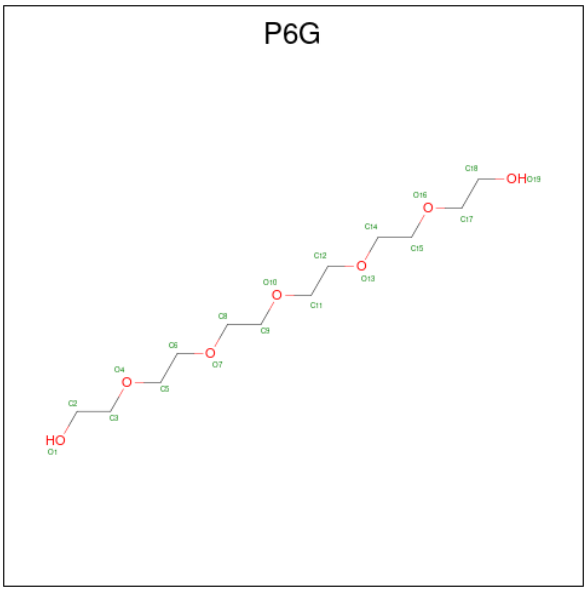
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	534	Total	C	N	O	S	0	0	1
			4159	2670	719	756	14			

- Molecule 2 is 1-[({2,4-BIS[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL}METHOXY)METHYL]-4-CARBAMOYLPYRIDINIUM (three-letter code: HLO) (formula: $C_{15}H_{17}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	15	5	4		
2	B	1	Total	C	N	O	0	0
			24	15	5	4		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 19 12 7	0	0

- Molecule 4 is water.

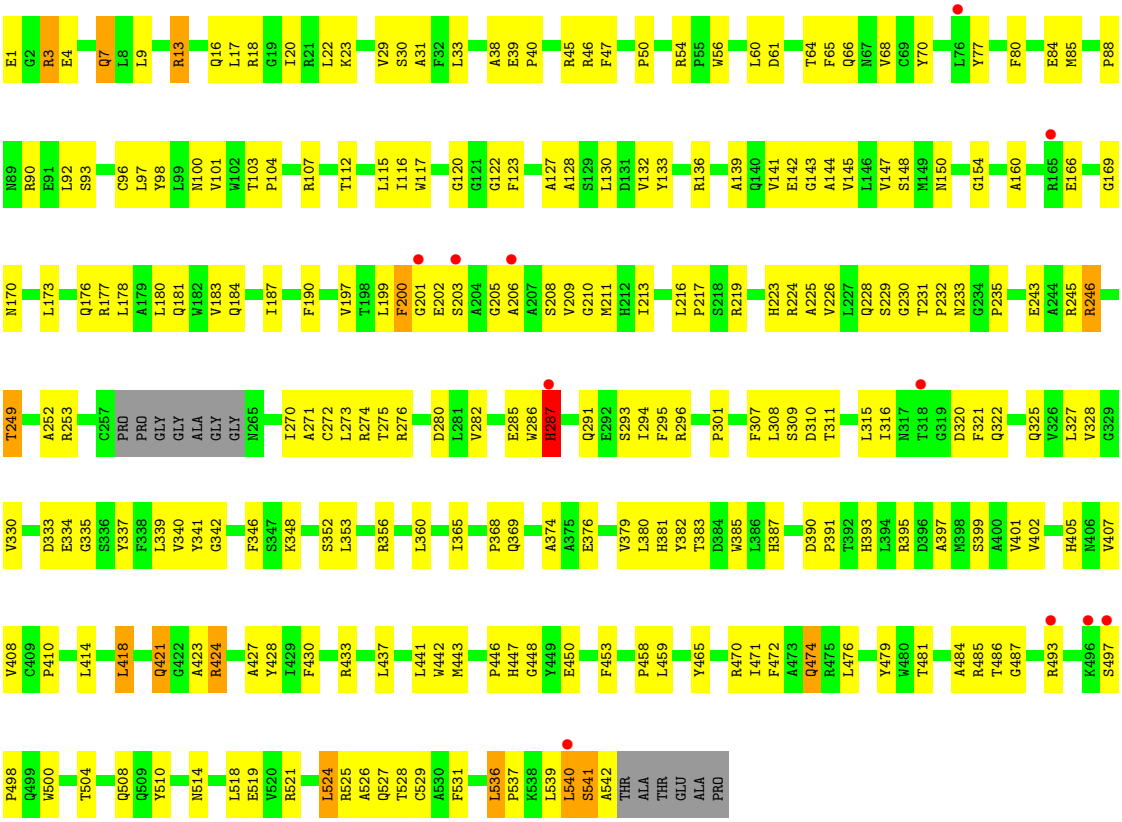
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	69	Total O 69 69	0	0

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.

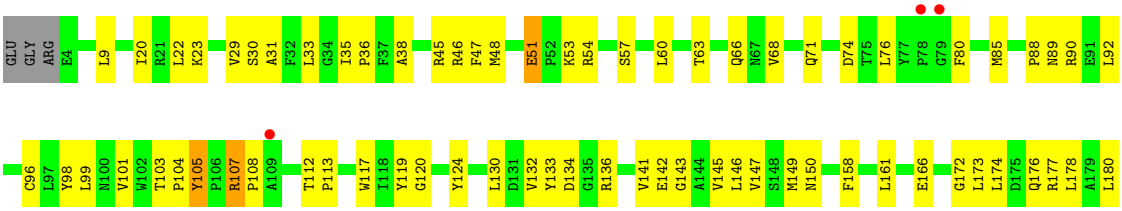
• Molecule 1: ACETYLCHOLINESTERASE

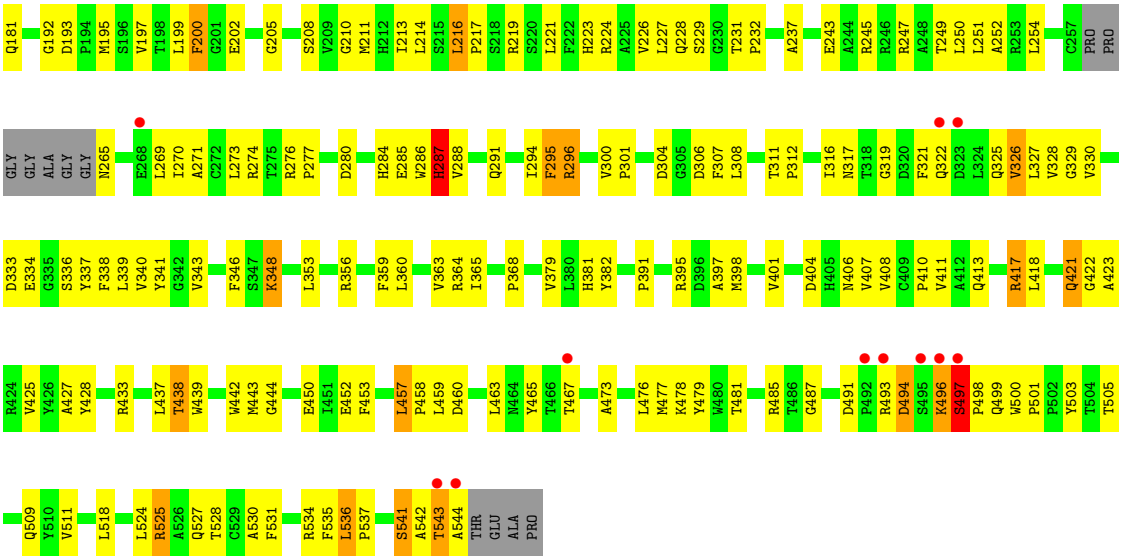
Chain A:



• Molecule 1: ACETYLCHOLINESTERASE

Chain B:




Q181 G192 D193 P194 M195 S196 V197 T198 L199 F200 G201 E202 G205 S208 V209 G210 M211 H212 T213 L214 S215 L216 P217 S218 R219 S220 L221 F222 H223 R224 A225 V226 L227 Q228 S229 G230 T231 P232 A237 E243 A244 R245 R246 R247 A248 T249 L250 L251 A252 R253 L254 C257 PRO PRO
GLY GLY ALA GLY GLY N265 E268 L269 I270 A271 C272 L273 R274 T275 R276 P277 D280 H284 E285 W286 H287 V288 Q291 I294 F295 R296 V300 P301 D304 G305 D306 F307 L308 T311 P312 I316 N317 T318 G319 D320 F321 Q322 D323 L324 Q325 V326 L327 V328 G329 V330
D333 E334 G335 S336 Y337 F338 L339 V340 Y341 G342 V343 F346 S347 K348 L353 R356 F359 L360 V363 R364 I365 P368 V379 L380 H381 Y382 P391 R395 D396 A397 M398 V401 D404 H405 N406 V407 V408 C409 P410 V411 A412 Q413 R417 L418 Q421 G422 A423
R424 V425 Y426 A427 Y428 R433 L437 T438 W439 W442 M443 G444 E450 I451 E452 F453 L457 P458 L459 D460 L463 N464 Y465 T466 T467 A473 L476 M477 K478 Y479 W480 T481 R485 T486 G487 D491 P492 R493 D494 S495 K496 S497 P498 Q499 W500 P501 P502 Y503 T504 T505
Q509 Y510 V511 L518 L524 R525 A526 Q527 T528 C529 A530 F531 R534 F535 L536 P537 S541 A542 T543 A544 THR GLU ALA PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.67Å 108.45Å 220.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.70 29.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.88-2.70) 100.0 (29.88-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.261 0.200 , 0.248	Depositor DCC
R_{free} test set	1011 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8565	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HLO, P6G

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	0.76	1/4300 (0.0%)	0.78	2/5875 (0.0%)
1	B	0.72	1/4282 (0.0%)	0.77	2/5853 (0.0%)
All	All	0.74	2/8582 (0.0%)	0.77	4/11728 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	413	GLN	CG-CD	6.34	1.65	1.51
1	A	272	CYS	CB-SG	-5.33	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	HIS	N-CA-CB	7.24	123.64	110.60
1	A	287	HIS	N-CA-CB	5.56	120.61	110.60
1	B	216	LEU	CA-CB-CG	-5.30	103.10	115.30
1	A	18	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	4177	0	4065	192	1
1	B	4159	0	4047	188	1
2	A	24	0	17	7	0
2	B	24	0	17	5	0
3	B	19	0	24	8	0
4	A	93	0	0	12	0
4	B	69	0	0	6	0
All	All	8565	0	8170	380	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (380) 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:197:VAL:H	1:B:223:HIS:CD2	1.75	1.03
1:B:452:GLU:HG3	4:B:2049:HOH:O	1.57	1.02
1:B:497:SER:HB2	1:B:498:PRO:CA	1.89	1.02
1:A:380:LEU:HB3	3:B:1546:P6G:H61	1.43	1.01
1:B:284:HIS:ND1	1:B:287:HIS:CE1	2.31	0.98
1:A:197:VAL:H	1:A:223:HIS:CD2	1.82	0.96
1:B:197:VAL:H	1:B:223:HIS:HD2	0.95	0.95
1:B:497:SER:HB2	1:B:498:PRO:HA	1.49	0.92
1:B:525:ARG:HH11	1:B:525:ARG:HG3	1.37	0.90
1:A:197:VAL:H	1:A:223:HIS:HD2	0.95	0.89
1:A:360:LEU:HD23	1:A:379:VAL:HG21	1.56	0.88
1:B:284:HIS:CG	1:B:287:HIS:CE1	2.62	0.88
1:B:119:TYR:HB2	4:B:2020:HOH:O	1.73	0.86
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.59	0.84
1:A:369:GLN:HB2	4:A:2056:HOH:O	1.77	0.83
1:B:197:VAL:N	1:B:223:HIS:HD2	1.77	0.82
1:B:479:TYR:OH	1:B:518:LEU:HD11	1.80	0.81
1:B:284:HIS:ND1	1:B:287:HIS:NE2	2.28	0.81
1:B:525:ARG:HH11	1:B:525:ARG:CG	1.94	0.81
1:A:213:ILE:O	1:A:219:ARG:HD3	1.79	0.80
1:B:360:LEU:HD22	1:B:379:VAL:HG11	1.64	0.80
1:B:497:SER:HB2	1:B:498:PRO:C	2.02	0.79
1:A:341:TYR:CD2	2:A:1543:HLO:H7C2	2.18	0.78
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.66	0.77
1:B:328:VAL:O	1:B:427:ALA:HA	1.86	0.76
1:A:128:ALA:HB1	1:A:148:SER:HB2	1.68	0.75
1:B:294:ILE:HG12	1:B:365:ILE:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:TRP:CH2	2:A:1543:HLO:H8C2	2.23	0.73
1:B:38:ALA:HB2	1:B:178:LEU:HD23	1.71	0.73
1:A:287:HIS:HB3	4:A:2053:HOH:O	1.90	0.72
1:B:284:HIS:CG	1:B:287:HIS:HE1	2.08	0.71
1:A:115:LEU:HD21	1:A:484:ALA:HB2	1.72	0.71
1:B:112:THR:HG21	1:B:143:GLY:O	1.90	0.71
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.73	0.71
1:B:326:VAL:HG21	1:B:418:LEU:HD13	1.73	0.70
1:A:380:LEU:HB3	3:B:1546:P6G:C6	2.20	0.70
1:B:525:ARG:HG3	1:B:525:ARG:NH1	2.06	0.70
1:B:304:ASP:OD2	1:B:306:ASP:HB3	1.91	0.70
1:A:245:ARG:O	1:A:249:THR:CG2	2.40	0.69
1:A:340:VAL:HG11	1:A:443:MET:CE	2.23	0.69
1:B:80:PHE:CE1	1:B:438:THR:OG1	2.47	0.68
1:B:45:ARG:O	1:B:48:MET:HB2	1.93	0.68
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.24	0.68
1:A:116:ILE:HD12	1:A:197:VAL:HG13	1.76	0.67
1:A:203:SER:HB2	1:A:447:HIS:NE2	2.10	0.66
1:B:433:ARG:NH2	1:B:439:TRP:O	2.28	0.66
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.78	0.66
1:A:103:THR:HG22	1:A:145:VAL:HG22	1.76	0.66
1:A:253:ARG:HD3	4:A:2045:HOH:O	1.95	0.66
1:A:321:PHE:HB2	1:A:423:ALA:HB2	1.78	0.66
1:B:210:GLY:HA3	1:B:232:PRO:HD3	1.77	0.65
1:B:322:GLN:HA	1:B:422:GLY:O	1.96	0.65
1:A:116:ILE:HD12	1:A:197:VAL:CG1	2.27	0.64
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.80	0.64
1:B:277:PRO:HG2	1:B:280:ASP:OD2	1.98	0.64
1:A:197:VAL:N	1:A:223:HIS:HD2	1.81	0.64
1:A:294:ILE:HD11	1:A:402:VAL:HG21	1.79	0.64
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.79	0.64
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.28	0.64
1:A:424:ARG:HD2	4:A:2073:HOH:O	1.99	0.63
1:A:122:GLY:O	1:A:123:PHE:HB2	1.99	0.63
1:A:245:ARG:O	1:A:249:THR:HG22	1.99	0.63
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.81	0.63
1:A:160:ALA:HB2	1:A:169:GLY:HA3	1.81	0.62
1:B:497:SER:CB	1:B:498:PRO:HA	2.26	0.62
1:A:341:TYR:CE2	2:A:1543:HLO:H7C2	2.33	0.62
1:B:141:VAL:HG21	1:B:459:LEU:CD2	2.30	0.62
1:A:101:VAL:HG22	1:A:147:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HA	1:A:228:GLN:O	1.99	0.62
1:A:340:VAL:CG1	1:A:443:MET:HE2	2.30	0.62
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.81	0.62
1:A:527:GLN:HE21	3:B:1546:P6G:H182	1.64	0.61
1:B:250:LEU:HG	1:B:288:VAL:HG12	1.82	0.61
1:B:497:SER:CB	1:B:498:PRO:CA	2.74	0.61
1:A:340:VAL:HG11	1:A:443:MET:HE2	1.81	0.61
1:A:45:ARG:HH22	1:A:54:ARG:HH22	1.47	0.61
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.83	0.61
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.35	0.60
1:B:180:LEU:HB3	1:B:221:LEU:HB3	1.83	0.60
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.83	0.59
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.35	0.59
1:B:45:ARG:NH1	1:B:51:GLU:HG2	2.17	0.59
1:B:101:VAL:HG22	1:B:147:VAL:HG22	1.82	0.59
1:A:470:ARG:O	1:A:474:GLN:HG2	2.03	0.59
1:B:103:THR:HG22	1:B:145:VAL:HG22	1.85	0.59
1:B:285:GLU:O	1:B:288:VAL:HG22	2.02	0.59
1:A:176:GLN:OE1	1:A:208:SER:HB3	2.02	0.59
1:A:245:ARG:O	1:A:249:THR:HG23	2.02	0.59
1:B:74:ASP:HB2	4:B:2018:HOH:O	2.03	0.58
1:A:393:HIS:HD2	4:A:2071:HOH:O	1.87	0.58
1:B:45:ARG:HH11	1:B:51:GLU:HG2	1.67	0.58
1:A:77:TYR:CZ	1:A:348:LYS:HG2	2.38	0.58
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.38	0.58
1:B:224:ARG:HD3	1:B:487:GLY:HA2	1.86	0.58
1:A:414:LEU:HG	1:A:418:LEU:HD22	1.86	0.57
1:A:68:VAL:HG13	1:A:127:ALA:HB2	1.86	0.57
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.85	0.57
1:B:254:LEU:HD13	1:B:287:HIS:ND1	2.20	0.57
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.40	0.57
1:A:85:MET:HE3	1:A:132:VAL:HG11	1.87	0.57
1:B:211:MET:HG3	1:B:232:PRO:HB3	1.87	0.57
1:B:88:PRO:HG3	1:B:92:LEU:HD21	1.86	0.56
1:A:17:LEU:HD23	1:A:60:LEU:HB3	1.88	0.56
1:A:46:ARG:HB3	1:A:274:ARG:HG2	1.87	0.56
1:A:128:ALA:HB1	1:A:148:SER:CB	2.36	0.56
1:A:271:ALA:O	1:A:275:THR:HG23	2.06	0.56
1:B:200:PHE:CB	1:B:226:VAL:HB	2.35	0.56
2:B:1545:HLO:H13	2:B:1545:HLO:H1	1.86	0.56
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:PRO:O	1:B:541:SER:HB3	2.05	0.56
1:B:265:ASN:ND2	4:B:2035:HOH:O	2.39	0.56
1:B:511:VAL:HG11	1:B:518:LEU:HD23	1.88	0.56
1:B:319:GLY:O	1:B:421:GLN:HG2	2.06	0.56
1:B:96:CYS:O	1:B:150:ASN:HB2	2.06	0.55
1:B:341:TYR:CE2	2:B:1545:HLO:H7C2	2.40	0.55
1:B:509:GLN:HB2	4:B:2058:HOH:O	2.05	0.55
1:A:542:ALA:HB1	1:B:544:ALA:N	2.22	0.55
1:B:224:ARG:HD3	1:B:487:GLY:CA	2.37	0.55
1:A:116:ILE:HD13	1:A:180:LEU:HD22	1.88	0.54
1:A:294:ILE:HD11	1:A:402:VAL:CG2	2.37	0.54
1:A:360:LEU:HD21	1:A:379:VAL:HG11	1.89	0.54
1:A:387:HIS:HB3	1:A:390:ASP:HB2	1.89	0.54
1:A:206:ALA:HB3	1:A:230:GLY:HA3	1.89	0.54
1:A:112:THR:HG21	1:A:143:GLY:O	2.08	0.54
1:B:341:TYR:CD2	2:B:1545:HLO:H7C2	2.42	0.54
1:B:381:HIS:HA	3:B:1546:P6G:H171	1.89	0.54
1:A:50:PRO:HB2	1:A:178:LEU:HD22	1.90	0.54
1:A:211:MET:HG3	1:A:232:PRO:HB3	1.90	0.54
1:A:200:PHE:CB	1:A:226:VAL:HB	2.38	0.54
1:B:473:ALA:O	1:B:477:MET:HG3	2.07	0.54
1:B:497:SER:HB3	1:B:499:GLN:HE21	1.73	0.54
1:A:235:PRO:HG3	1:A:405:HIS:CE1	2.43	0.53
1:A:450:GLU:OE1	1:A:450:GLU:N	2.37	0.53
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.43	0.53
1:A:328:VAL:O	1:A:427:ALA:HA	2.08	0.53
1:B:316:ILE:O	1:B:421:GLN:NE2	2.41	0.53
1:A:166:GLU:HB2	1:A:270:ILE:HD13	1.89	0.53
1:B:22:LEU:HB3	1:B:136:ARG:HH21	1.73	0.53
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.89	0.53
1:A:527:GLN:HG3	3:B:1546:P6G:H182	1.90	0.53
1:B:31:ALA:HB1	1:B:33:LEU:HD21	1.89	0.53
1:B:172:GLY:O	1:B:176:GLN:HG3	2.08	0.53
1:A:3:ARG:HA	1:A:3:ARG:HH11	1.73	0.53
1:A:107:ARG:HD2	1:A:190:PHE:HA	1.90	0.53
1:B:535:PHE:CD2	3:B:1546:P6G:H82	2.43	0.53
1:A:29:VAL:HG21	1:A:136:ARG:HB2	1.91	0.53
1:A:340:VAL:HG11	1:A:443:MET:HE1	1.91	0.53
1:A:339:LEU:HD11	1:A:399:SER:HA	1.90	0.52
1:A:524:LEU:O	1:A:525:ARG:C	2.48	0.52
1:A:139:ALA:HA	1:A:144:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.74	0.52
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.45	0.52
1:B:404:ASP:HA	1:B:408:VAL:HB	1.90	0.52
1:A:16:GLN:HG2	4:A:2002:HOH:O	2.08	0.52
1:A:231:THR:HB	1:A:233:ASN:OD1	2.10	0.52
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.92	0.51
1:A:541:SER:O	1:A:542:ALA:CB	2.58	0.51
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.92	0.51
1:B:252:ALA:HA	1:B:273:LEU:HD21	1.92	0.51
1:B:284:HIS:HD1	1:B:287:HIS:HE2	1.57	0.51
1:B:36:PRO:HB2	1:B:53:LYS:HD3	1.91	0.51
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.40	0.51
1:B:254:LEU:HD22	1:B:287:HIS:ND1	2.26	0.51
1:A:274:ARG:HD3	4:A:2047:HOH:O	2.09	0.51
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.40	0.51
1:B:501:PRO:HG2	1:B:509:GLN:HB3	1.92	0.51
1:A:20:ILE:HG23	1:A:31:ALA:HB3	1.93	0.51
1:A:38:ALA:HB2	1:A:178:LEU:HD23	1.92	0.51
1:A:210:GLY:HA2	1:A:213:ILE:HD12	1.93	0.51
1:A:540:LEU:O	1:A:542:ALA:N	2.41	0.50
1:A:96:CYS:O	1:A:150:ASN:HB2	2.10	0.50
1:B:99:LEU:HA	1:B:149:MET:HA	1.93	0.50
1:B:382:TYR:CD1	1:B:401:VAL:HG22	2.46	0.50
1:A:316:ILE:O	1:A:421:GLN:NE2	2.45	0.49
1:A:100:ASN:O	1:A:147:VAL:HA	2.12	0.49
1:A:249:THR:O	1:A:252:ALA:HB3	2.12	0.49
1:B:48:MET:SD	1:B:166:GLU:HA	2.52	0.49
1:B:30:SER:HB2	1:B:103:THR:OG1	2.12	0.49
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.28	0.49
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.48	0.49
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.93	0.49
1:A:142:GLU:CB	1:A:481:THR:HG21	2.43	0.49
1:A:395:ARG:CZ	1:A:442:TRP:HB2	2.43	0.49
1:A:374:ALA:HB1	1:A:536:LEU:HD21	1.95	0.48
1:B:327:LEU:HD11	1:B:500:TRP:CH2	2.48	0.48
1:B:527:GLN:O	1:B:530:ALA:HB3	2.13	0.48
1:A:339:LEU:HD11	1:A:399:SER:CA	2.42	0.48
1:B:202:GLU:HA	1:B:228:GLN:O	2.12	0.48
1:A:22:LEU:HB2	1:A:29:VAL:HG23	1.95	0.48
1:A:46:ARG:NH1	1:A:276:ARG:O	2.41	0.48
1:A:77:TYR:CE1	1:A:348:LYS:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PHE:HE1	1:B:173:LEU:HG	1.78	0.48
1:B:237:ALA:O	1:B:301:PRO:HD2	2.14	0.48
1:B:359:PHE:O	1:B:363:VAL:HG23	2.14	0.48
1:A:84:GLU:HA	1:A:84:GLU:OE1	2.13	0.48
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.95	0.48
1:A:393:HIS:CD2	4:A:2071:HOH:O	2.62	0.48
1:A:414:LEU:O	1:A:418:LEU:HB2	2.14	0.47
1:B:146:LEU:HD23	1:B:147:VAL:N	2.29	0.47
1:A:504:THR:O	1:A:508:GLN:N	2.39	0.47
1:B:479:TYR:OH	1:B:518:LEU:CD1	2.58	0.47
1:B:243:GLU:O	1:B:247:ARG:HG3	2.15	0.47
1:A:282:VAL:O	1:A:285:GLU:HG2	2.14	0.47
1:A:536:LEU:N	1:A:537:PRO:CD	2.78	0.47
1:B:89:ASN:O	1:B:90:ARG:NH1	2.45	0.47
1:B:536:LEU:HD22	1:B:536:LEU:HA	1.71	0.47
1:A:181:GLN:O	1:A:184:GLN:HB2	2.15	0.47
1:A:525:ARG:HD3	4:A:2087:HOH:O	2.15	0.47
1:A:341:TYR:CD2	2:A:1543:HLO:C7	2.94	0.47
1:A:352:SER:O	1:A:395:ARG:HG3	2.15	0.47
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.95	0.47
1:B:330:VAL:HG11	1:B:408:VAL:HA	1.96	0.47
1:B:493:ARG:O	1:B:494:ASP:HB2	2.14	0.47
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.48	0.47
1:B:161:LEU:HD12	1:B:270:ILE:HG13	1.96	0.47
1:A:120:GLY:HA2	1:A:205:GLY:H	1.80	0.47
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.97	0.47
1:A:77:TYR:CG	1:A:348:LYS:HD3	2.50	0.47
1:A:433:ARG:CZ	1:A:437:LEU:HD23	2.46	0.46
1:A:80:PHE:CE1	1:A:348:LYS:HE3	2.50	0.46
1:A:407:VAL:C	1:A:410:PRO:HD2	2.35	0.46
1:A:116:ILE:CD1	1:A:197:VAL:HG13	2.44	0.46
1:A:430:PHE:CD2	1:A:450:GLU:HB2	2.51	0.46
1:B:271:ALA:O	1:B:274:ARG:HB2	2.15	0.46
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.51	0.46
1:A:330:VAL:HG11	1:A:408:VAL:HA	1.98	0.46
1:A:360:LEU:CD2	1:A:379:VAL:HG11	2.45	0.46
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.15	0.46
1:B:518:LEU:HD12	4:B:2061:HOH:O	2.15	0.46
1:A:33:LEU:HD22	1:A:65:PHE:CE1	2.50	0.46
1:A:287:HIS:CB	4:A:2053:HOH:O	2.57	0.46
1:A:397:ALA:O	1:A:401:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD11	1:A:225:ALA:CB	2.45	0.45
1:A:528:THR:O	1:A:531:PHE:HB3	2.16	0.45
1:B:339:LEU:O	1:B:343:VAL:HB	2.15	0.45
1:A:80:PHE:O	1:A:84:GLU:HG2	2.16	0.45
1:A:537:PRO:O	1:A:540:LEU:HD23	2.17	0.45
1:B:214:LEU:HD11	1:B:316:ILE:HG23	1.98	0.45
1:B:317:ASN:HA	1:B:417:ARG:HH11	1.82	0.45
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.98	0.45
1:A:428:TYR:HB3	1:A:500:TRP:CZ2	2.51	0.45
1:A:70:TYR:HD2	1:A:282:VAL:HG21	1.80	0.45
1:B:528:THR:O	1:B:531:PHE:HB3	2.16	0.45
1:A:7:GLN:HG2	4:A:2023:HOH:O	2.16	0.45
1:A:374:ALA:HA	1:A:539:LEU:HD23	1.98	0.45
1:A:380:LEU:HD11	1:B:534:ARG:HB2	1.98	0.45
1:A:334:GLU:CD	1:A:407:VAL:HG11	2.37	0.45
1:A:485:ARG:HB3	1:A:486:THR:HG23	1.99	0.45
1:B:22:LEU:HD13	1:B:136:ARG:NH2	2.32	0.45
1:B:525:ARG:CG	1:B:525:ARG:NH1	2.63	0.45
1:A:9:LEU:HB3	4:A:2002:HOH:O	2.17	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.98	0.44
1:A:321:PHE:CB	1:A:423:ALA:HB2	2.44	0.44
1:A:333:ASP:O	1:A:446:PRO:HA	2.16	0.44
1:A:339:LEU:HD11	1:A:399:SER:N	2.32	0.44
2:A:1543:HLO:H8C1	2:A:1543:HLO:C1	2.47	0.44
1:B:542:ALA:O	1:B:543:THR:OG1	2.30	0.44
1:B:346:PHE:HE2	1:B:395:ARG:HG2	1.81	0.44
1:B:382:TYR:HB3	1:B:397:ALA:HB1	1.99	0.44
1:B:213:ILE:O	1:B:219:ARG:HD3	2.16	0.44
1:B:317:ASN:HA	1:B:417:ARG:NH1	2.33	0.44
1:A:183:VAL:HG13	1:A:187:ILE:HB	1.98	0.44
1:B:193:ASP:C	1:B:195:MET:H	2.20	0.44
1:B:105:TYR:C	1:B:105:TYR:CD2	2.90	0.44
1:A:1:GLU:N	1:A:4:GLU:OE1	2.42	0.44
1:A:356:ARG:NH2	1:A:383:THR:OG1	2.43	0.44
1:B:53:LYS:HG3	1:B:54:ARG:O	2.17	0.44
1:B:499:GLN:O	1:B:501:PRO:HD3	2.16	0.44
1:A:294:ILE:CD1	1:A:402:VAL:HG21	2.47	0.44
1:B:120:GLY:HA2	1:B:205:GLY:H	1.83	0.44
1:A:310:ASP:OD1	1:A:311:THR:N	2.45	0.43
1:A:479:TYR:OH	1:A:518:LEU:HG	2.18	0.43
1:A:527:GLN:HG3	3:B:1546:P6G:C18	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ARG:O	1:B:249:THR:OG1	2.24	0.43
1:B:333:ASP:O	1:B:334:GLU:C	2.56	0.43
1:B:338:PHE:CE2	2:B:1545:HLO:H3	2.52	0.43
1:B:498:PRO:HG2	1:B:518:LEU:O	2.18	0.43
1:B:284:HIS:CB	1:B:287:HIS:CE1	3.00	0.43
1:B:407:VAL:C	1:B:410:PRO:HD2	2.38	0.43
1:B:20:ILE:HB	1:B:63:THR:HB	2.00	0.43
1:B:46:ARG:HD3	1:B:47:PHE:CZ	2.54	0.43
1:B:336:SER:O	1:B:337:TYR:C	2.57	0.43
1:A:474:GLN:HE21	1:A:474:GLN:HB3	1.62	0.43
1:B:340:VAL:CG1	1:B:443:MET:CE	2.97	0.43
1:A:381:HIS:HA	3:B:1546:P6G:H31	2.00	0.43
1:A:430:PHE:HE2	1:A:476:LEU:CD1	2.31	0.43
1:B:428:TYR:HA	1:B:511:VAL:O	2.18	0.43
1:A:202:GLU:OE2	1:A:448:GLY:HA2	2.18	0.43
1:B:146:LEU:HD23	1:B:146:LEU:C	2.39	0.43
1:B:202:GLU:HG3	1:B:450:GLU:OE2	2.19	0.43
1:B:68:VAL:CG1	1:B:71:GLN:NE2	2.82	0.43
1:B:36:PRO:HD3	1:B:60:LEU:HD21	2.01	0.43
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.79	0.43
1:B:132:VAL:HG12	1:B:452:GLU:HG2	2.00	0.43
1:A:321:PHE:O	1:A:423:ALA:HA	2.19	0.42
1:A:380:LEU:HD11	1:B:534:ARG:CB	2.49	0.42
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.84	0.42
1:A:235:PRO:HB2	1:A:296:ARG:NH2	2.34	0.42
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.54	0.42
1:A:541:SER:O	1:A:542:ALA:HB3	2.19	0.42
1:B:35:ILE:O	1:B:98:TYR:HA	2.19	0.42
1:B:425:VAL:O	1:B:503:TYR:N	2.52	0.42
1:A:116:ILE:HA	1:A:147:VAL:O	2.19	0.42
1:A:226:VAL:HA	1:A:327:LEU:O	2.18	0.42
1:A:335:GLY:HA3	1:A:399:SER:O	2.18	0.42
1:B:166:GLU:CB	1:B:274:ARG:HH22	2.32	0.42
1:B:321:PHE:HB3	1:B:423:ALA:HB2	2.02	0.42
1:B:326:VAL:HG21	1:B:418:LEU:CD1	2.45	0.42
1:A:39:GLU:O	1:A:40:PRO:C	2.57	0.42
1:A:173:LEU:HB3	1:A:307:PHE:CZ	2.55	0.42
1:B:231:THR:HG21	1:B:411:VAL:HA	2.01	0.42
1:B:124:TYR:CD1	1:B:124:TYR:C	2.93	0.42
1:B:433:ARG:HG3	1:B:444:GLY:O	2.19	0.42
1:A:88:PRO:CG	1:A:92:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:CG1	1:A:225:ALA:HB1	2.50	0.42
1:A:232:PRO:HD2	1:A:414:LEU:HD13	2.02	0.42
1:A:382:TYR:CD1	1:A:401:VAL:HG22	2.54	0.42
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.01	0.42
2:A:1543:HLO:C13	2:A:1543:HLO:H1	2.49	0.42
1:B:398:MET:HE3	1:B:398:MET:HA	2.02	0.42
1:A:117:TRP:CZ3	1:A:201:GLY:HA2	2.55	0.42
1:B:117:TRP:HA	1:B:200:PHE:O	2.20	0.42
1:B:214:LEU:HD21	1:B:316:ILE:HG22	2.02	0.42
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.55	0.42
1:A:327:LEU:HD11	1:A:500:TRP:CZ2	2.55	0.41
1:B:80:PHE:CD1	1:B:348:LYS:HE2	2.55	0.41
1:B:364:ARG:O	1:B:368:PRO:HA	2.20	0.41
1:A:309:SER:OG	1:A:315:LEU:HD21	2.20	0.41
1:A:376:GLU:OE2	1:A:380:LEU:CD2	2.68	0.41
1:A:30:SER:HB2	1:A:103:THR:OG1	2.20	0.41
1:A:525:ARG:O	1:A:526:ALA:C	2.57	0.41
1:B:22:LEU:HB2	1:B:29:VAL:HG23	2.02	0.41
1:B:311:THR:O	1:B:312:PRO:C	2.58	0.41
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.20	0.41
1:B:85:MET:CE	1:B:132:VAL:HG11	2.50	0.41
1:A:224:ARG:HD3	1:A:487:GLY:CA	2.50	0.41
1:A:346:PHE:HE2	1:A:395:ARG:HG2	1.86	0.41
1:B:89:ASN:O	1:B:90:ARG:HG2	2.21	0.41
1:B:107:ARG:HE	1:B:107:ARG:HB2	1.38	0.41
1:B:276:ARG:O	1:B:277:PRO:C	2.59	0.41
1:A:60:LEU:HD23	1:A:61:ASP:C	2.41	0.41
1:B:329:GLY:HA3	1:B:428:TYR:CD2	2.55	0.41
1:A:233:ASN:OD1	1:A:233:ASN:N	2.52	0.41
1:A:497:SER:HA	1:A:498:PRO:HD3	1.94	0.41
1:B:134:ASP:OD2	1:B:136:ARG:HD2	2.20	0.41
1:B:177:ARG:CZ	1:B:307:PHE:CE2	3.03	0.41
1:B:284:HIS:CE1	1:B:287:HIS:CE1	3.05	0.41
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.84	0.41
1:B:251:LEU:HA	1:B:254:LEU:HD12	2.03	0.41
1:B:453:PHE:HB3	1:B:476:LEU:CD1	2.51	0.41
1:A:3:ARG:HH11	1:A:3:ARG:CG	2.34	0.41
1:A:142:GLU:HB3	1:A:481:THR:HG21	2.03	0.41
1:A:199:LEU:O	1:A:226:VAL:N	2.49	0.41
1:A:293:SER:CB	1:A:296:ARG:HB2	2.51	0.41
1:B:295:PHE:CE2	1:B:338:PHE:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.51	0.41
1:A:229:SER:O	1:A:447:HIS:HE1	2.04	0.41
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.56	0.41
1:B:340:VAL:HG11	1:B:443:MET:CE	2.51	0.41
1:B:145:VAL:HG21	1:B:192:GLY:CA	2.52	0.40
1:A:85:MET:HE3	1:A:132:VAL:CG1	2.51	0.40
1:A:130:LEU:HB2	1:A:133:TYR:CD2	2.56	0.40
1:A:208:SER:O	1:A:209:VAL:C	2.57	0.40
1:B:36:PRO:CD	1:B:60:LEU:HD21	2.52	0.40
1:B:76:LEU:HD22	1:B:341:TYR:CD2	2.56	0.40
1:B:142:GLU:HB3	1:B:481:THR:HG21	2.02	0.40
1:B:199:LEU:O	1:B:226:VAL:N	2.54	0.40
1:B:229:SER:OG	1:B:334:GLU:OE2	2.27	0.40
1:A:47:PHE:CE2	1:A:273:LEU:HB3	2.57	0.40
2:A:1543:HLO:H1	2:A:1543:HLO:H13	2.03	0.40
1:B:300:VAL:HB	1:B:301:PRO:HD2	2.03	0.40
1:A:365:ILE:O	1:A:368:PRO:HD3	2.21	0.40
1:A:385:TRP:CD1	1:B:530:ALA:HB2	2.57	0.40
1:A:525:ARG:HB2	1:A:529:CYS:SG	2.62	0.40
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.83	0.40
1:B:177:ARG:NH2	1:B:307:PHE:CE2	2.89	0.40
1:B:457:LEU:N	1:B:458:PRO:CD	2.85	0.40
1:A:56:TRP:NE1	1:A:60:LEU:HB2	2.36	0.40
1:A:123:PHE:O	1:A:154:GLY:N	2.29	0.40
1:B:338:PHE:HE2	2:B:1545:HLO:H3	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH1	1:B:57:SER:O[2_555]	2.14	0.06

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	531/548 (97%)	491 (92%)	37 (7%)	3 (1%)	25 50
1	B	530/548 (97%)	492 (93%)	33 (6%)	5 (1%)	17 40
All	All	1061/1096 (97%)	983 (93%)	70 (7%)	8 (1%)	19 43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	494	ASP
1	B	497	SER
1	A	541	SER
1	B	541	SER
1	A	493	ARG
1	B	496	LYS
1	B	543	THR
1	A	342	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	439/446 (98%)	411 (94%)	28 (6%)	17 39
1	B	438/446 (98%)	409 (93%)	29 (7%)	16 38
All	All	877/892 (98%)	820 (94%)	57 (6%)	17 38

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	GLN
1	A	13	ARG
1	A	23	LYS
1	A	64	THR

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Mol	Chain	Res	Type
1	A	93	SER
1	A	200	PHE
1	A	216	LEU
1	A	246	ARG
1	A	249	THR
1	A	280	ASP
1	A	287	HIS
1	A	291	GLN
1	A	295	PHE
1	A	320	ASP
1	A	322	GLN
1	A	337	TYR
1	A	418	LEU
1	A	421	GLN
1	A	424	ARG
1	A	441	LEU
1	A	471	ILE
1	A	474	GLN
1	A	514	ASN
1	A	519	GLU
1	A	524	LEU
1	A	536	LEU
1	A	540	LEU
1	B	9	LEU
1	B	23	LYS
1	B	51	GLU
1	B	105	TYR
1	B	107	ARG
1	B	181	GLN
1	B	200	PHE
1	B	216	LEU
1	B	286	TRP
1	B	287	HIS
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	326	VAL
1	B	348	LYS
1	B	356	ARG
1	B	417	ARG
1	B	421	GLN
1	B	437	LEU

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Mol	Chain	Res	Type
1	B	438	THR
1	B	457	LEU
1	B	467	THR
1	B	478	LYS
1	B	496	LYS
1	B	497	SER
1	B	505	THR
1	B	524	LEU
1	B	525	ARG
1	B	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	223	HIS
1	A	291	GLN
1	A	393	HIS
1	A	421	GLN
1	A	464	ASN
1	A	474	GLN
1	B	223	HIS
1	B	291	GLN
1	B	499	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)

3 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	HLO	B	1545	-	21,25,25	0.74	1 (4%)	22,32,32	2.12	2 (9%)
2	HLO	A	1543	-	21,25,25	0.87	1 (4%)	22,32,32	1.94	3 (13%)
3	P6G	B	1546	-	18,18,18	1.78	5 (27%)	17,17,17	1.98	9 (52%)

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	HLO	B	1545	-	-	7/15/16/16	0/2/2/2
2	HLO	A	1543	-	-	7/15/16/16	0/2/2/2
3	P6G	B	1546	-	-	8/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1546	P6G	C9-C8	-3.06	1.33	1.49
3	B	1546	P6G	C17-C18	-2.99	1.33	1.49
3	B	1546	P6G	C3-C2	-2.94	1.33	1.49
3	B	1546	P6G	C15-C14	-2.86	1.34	1.49
3	B	1546	P6G	C6-C5	-2.86	1.34	1.49
2	A	1543	HLO	C2-N2	-2.83	1.34	1.37
2	B	1545	HLO	C2-N2	-2.19	1.35	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1545	HLO	O4-N5-C22	7.14	124.46	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1543	HLO	O4-N5-C22	6.49	123.32	111.86
2	B	1545	HLO	O1-N1-C1	5.60	121.75	111.86
2	A	1543	HLO	O1-N1-C1	3.86	118.67	111.86
3	B	1546	P6G	O13-C14-C15	3.42	125.82	110.39
2	A	1543	HLO	C2-C1-N1	2.82	123.21	117.75
3	B	1546	P6G	O16-C15-C14	2.82	123.12	110.39
3	B	1546	P6G	O4-C3-C2	2.35	120.39	110.07
3	B	1546	P6G	O7-C6-C5	2.24	120.51	110.39
3	B	1546	P6G	O7-C8-C9	2.22	120.41	110.39
3	B	1546	P6G	C5-O4-C3	2.20	122.81	113.29
3	B	1546	P6G	C8-O7-C6	2.15	122.58	113.29
3	B	1546	P6G	O16-C17-C18	2.12	119.38	110.07
3	B	1546	P6G	O4-C5-C6	2.06	119.70	110.39

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1543	HLO	O2-C8-N3-C9
2	A	1543	HLO	N1-C1-C2-N2
2	A	1543	HLO	N1-C1-C2-C3
2	B	1545	HLO	O2-C8-N3-C9
2	B	1545	HLO	N1-C1-C2-N2
2	B	1545	HLO	N1-C1-C2-C3
2	B	1545	HLO	N5-C22-C4-C3
2	A	1543	HLO	N5-C22-C4-C3
2	A	1543	HLO	N5-C22-C4-C5
2	B	1545	HLO	N5-C22-C4-C5
3	B	1546	P6G	O7-C8-C9-O10
3	B	1546	P6G	O4-C5-C6-O7
3	B	1546	P6G	O13-C14-C15-O16
2	A	1543	HLO	N3-C8-O2-C7
2	A	1543	HLO	N2-C7-O2-C8
2	B	1545	HLO	N3-C8-O2-C7
3	B	1546	P6G	C12-C11-O10-C9
3	B	1546	P6G	C6-C5-O4-C3
3	B	1546	P6G	C2-C3-O4-C5
2	B	1545	HLO	N2-C7-O2-C8
3	B	1546	P6G	O10-C11-C12-O13
3	B	1546	P6G	C18-C17-O16-C15

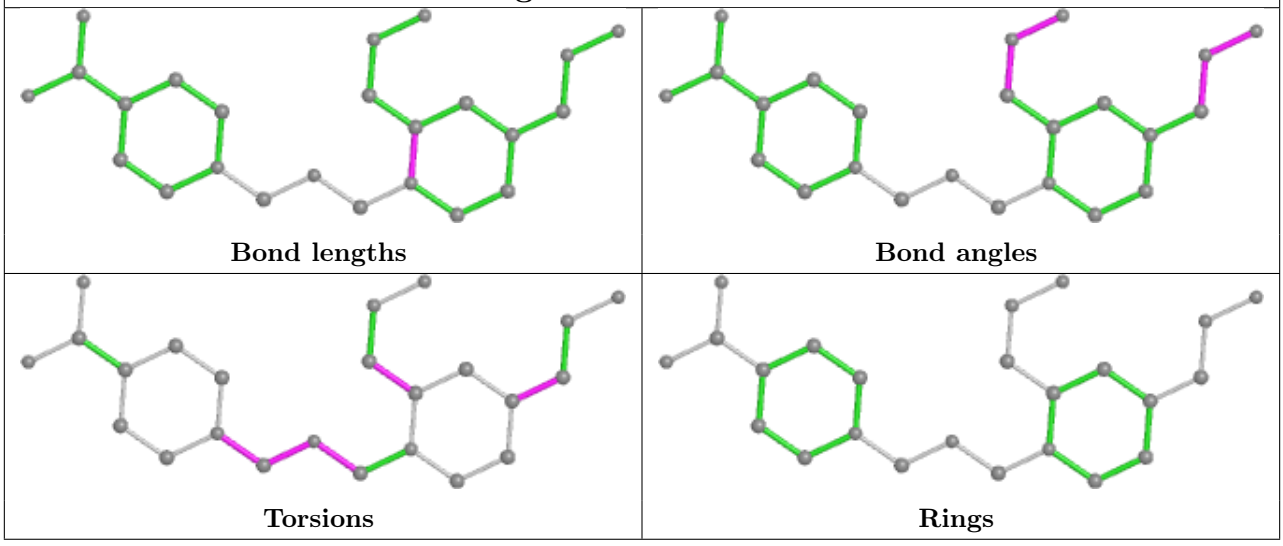
There are no ring outliers.

3 monomers are involved in 20 short contacts:

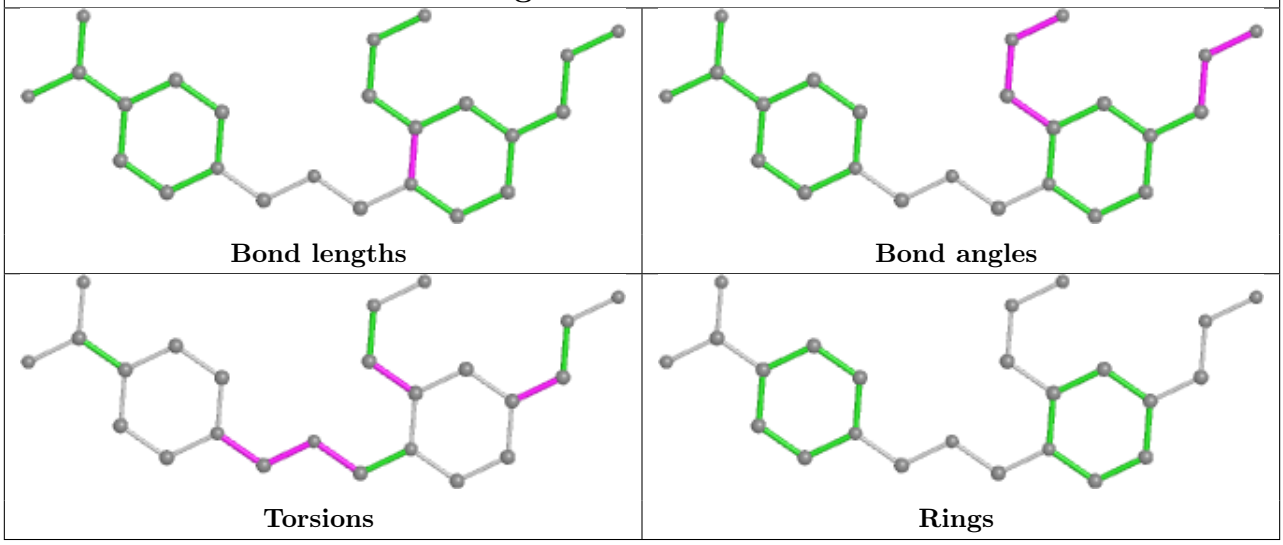
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1545	HLO	5	0
2	A	1543	HLO	7	0
3	B	1546	P6G	8	0

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.

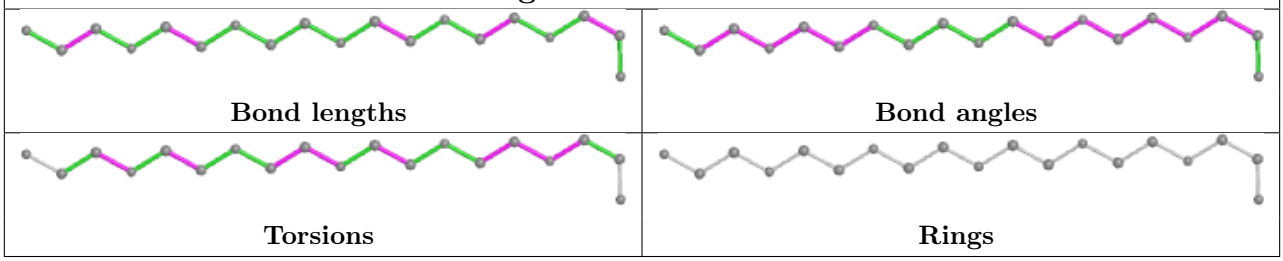
Ligand HLO B 1545



Ligand HLO A 1543



Ligand P6G B 1546



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

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, 95^{th} 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	535/548 (97%)	-0.18	11 (2%)	63	65	19, 34, 55, 78	0
1	B	534/548 (97%)	-0.12	14 (2%)	56	57	23, 38, 57, 75	0
All	All	1069/1096 (97%)	-0.15	25 (2%)	60	62	19, 36, 56, 78	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	ALA	7.2
1	A	496	LYS	4.2
1	A	203	SER	3.4
1	B	78	PRO	3.4
1	A	493	ARG	3.3
1	B	543	THR	3.2
1	B	79	GLY	3.1
1	B	495	SER	3.1
1	B	497	SER	3.0
1	B	496	LYS	2.9
1	B	268	GLU	2.8
1	A	540	LEU	2.7
1	B	492	PRO	2.6
1	A	206	ALA	2.5
1	A	497	SER	2.4
1	A	287	HIS	2.4
1	A	165	ARG	2.3
1	B	493	ARG	2.2
1	A	201	GLY	2.2
1	A	76	LEU	2.2
1	B	109	ALA	2.2
1	A	318	THR	2.2
1	B	467	THR	2.1
1	B	323	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLN	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)

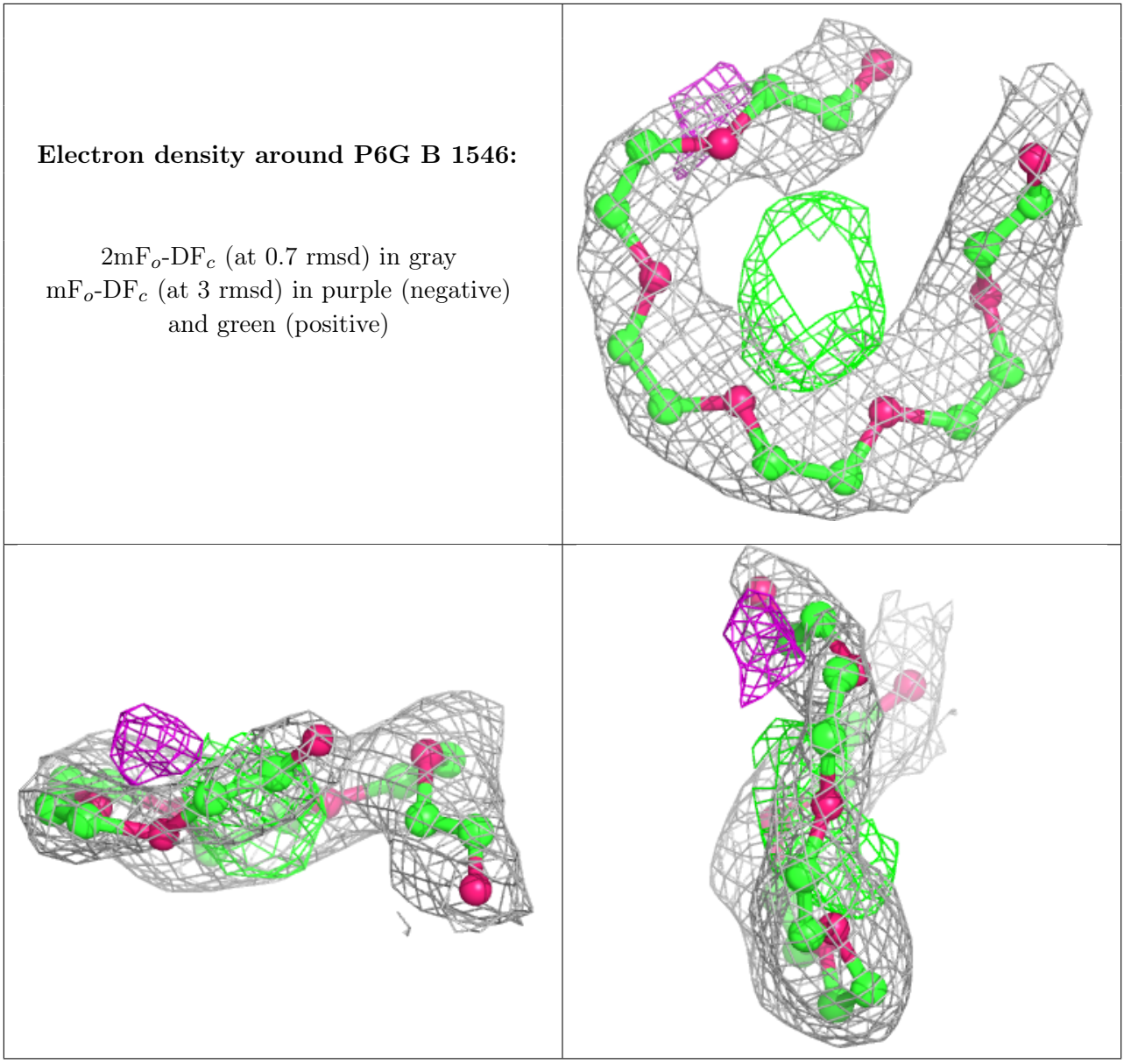
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P6G	B	1546	19/19	0.90	0.23	47,52,62,62	0
2	HLO	B	1545	24/24	0.93	0.28	41,51,60,60	24
2	HLO	A	1543	24/24	0.94	0.19	32,42,55,58	24

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.

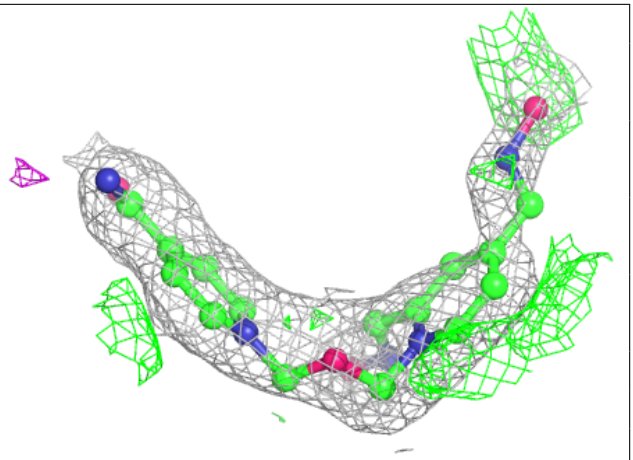
Electron density around P6G B 1546:

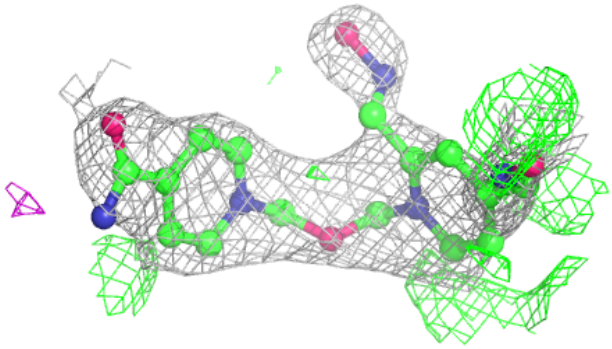
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

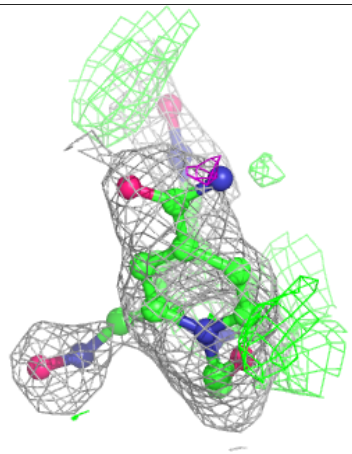


Electron density around HLO B 1545:

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

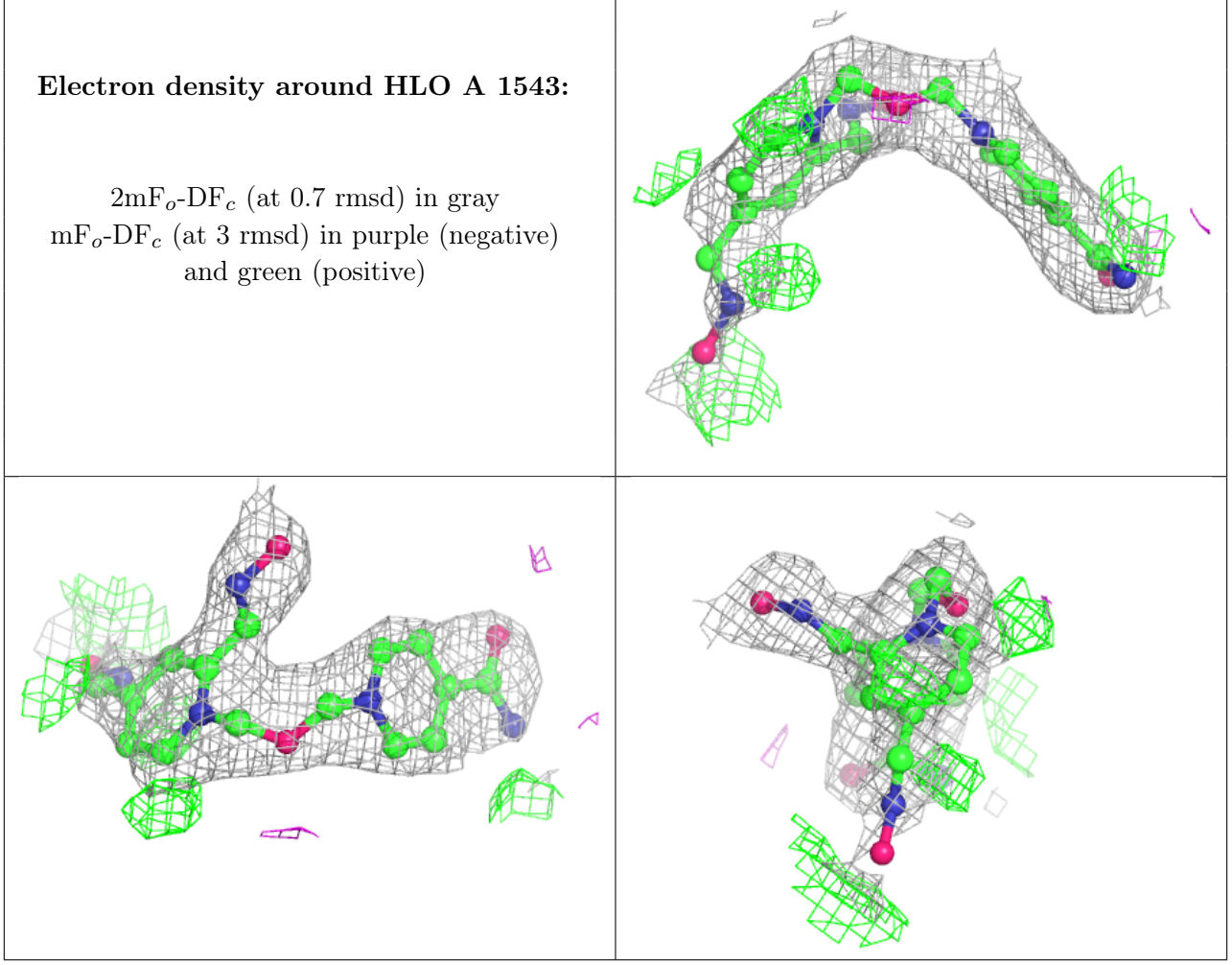






Electron density around HLO A 1543:

$2mF_o$-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.