Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 10:51 PM EDT

PDB ID	:	1HPZ
Title	:	HUMAN IMMUNODEFICIENCY VIRUS TYPE 1
Authors	:	Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on	:	2000-12-13
Resolution	:	3.00 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:

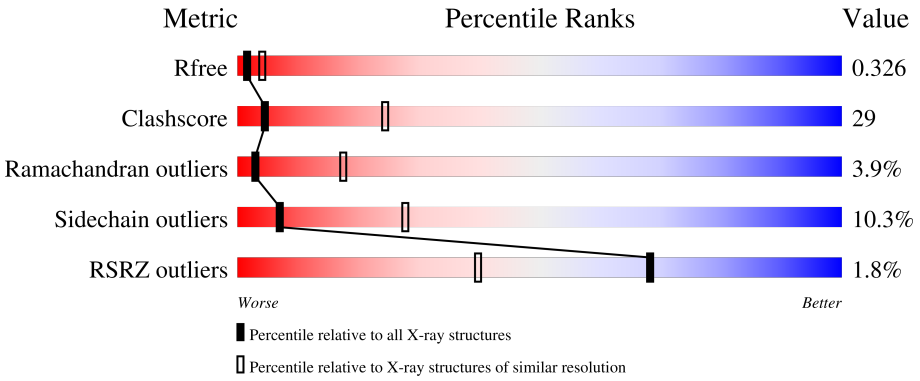
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	560	2% 49% 44% 6%
2	B	430	2% 50% 45% 5%

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	AAP	A	561	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7821 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 POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4377	2826	725	819	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

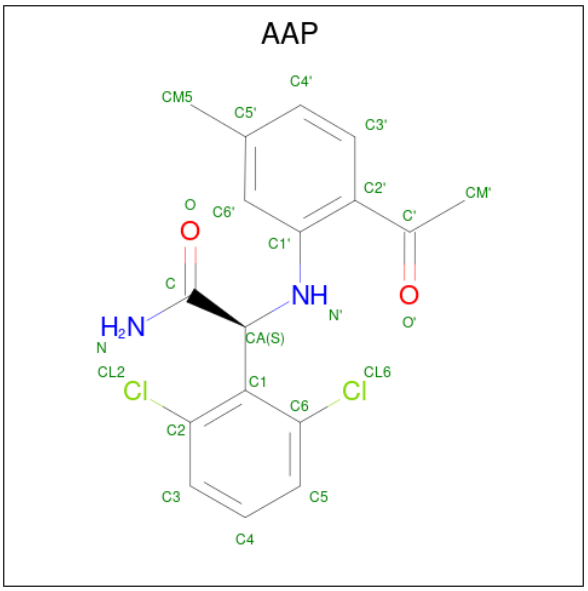
- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3421	2224	561	630	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	ASN	LYS	engineered mutation	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is ALPHA-(2,6-DICHLOROPHENYL)-ALPHA-(2-ACETYL-5-METHYLANILINO)ACETAMIDE (three-letter code: AAP) (formula: $C_{17}H_{16}Cl_2N_2O_2$).



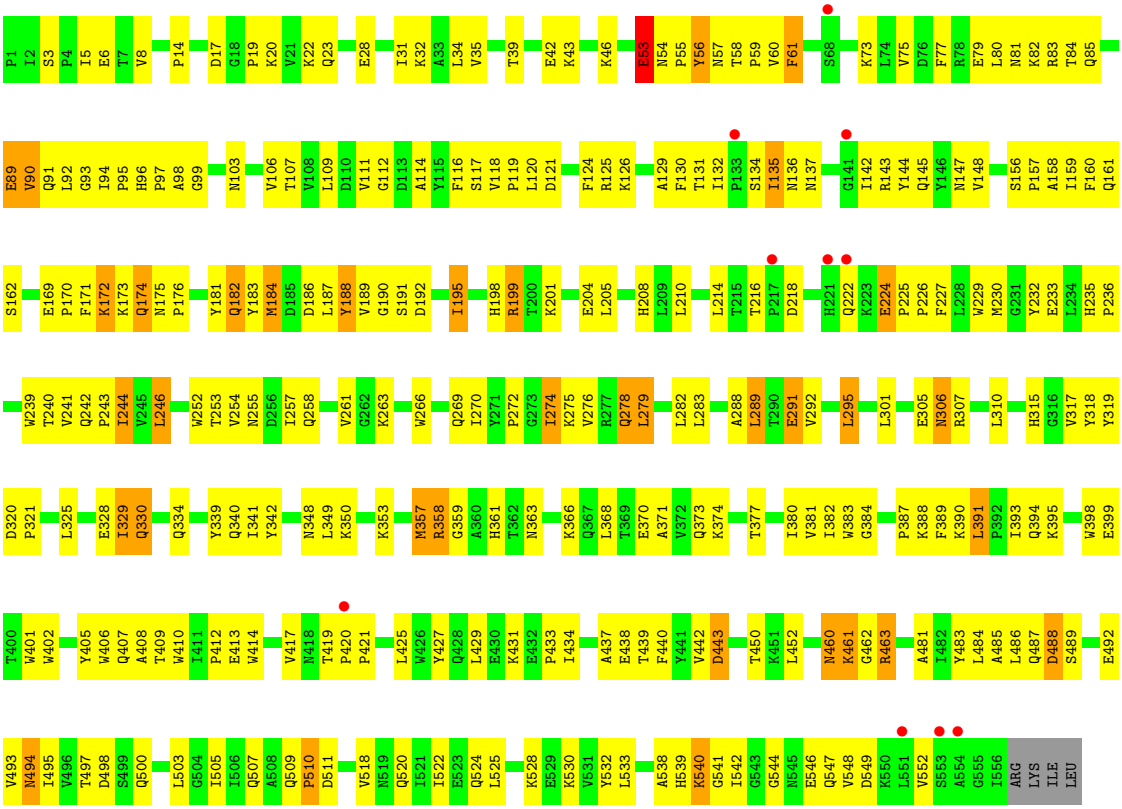
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	23	17	2	2	2	0	0

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.

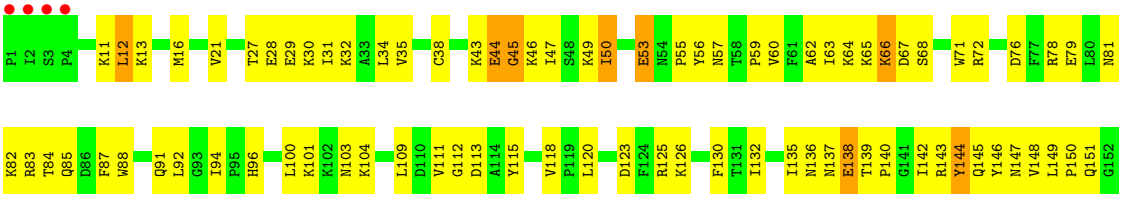
• Molecule 1: POL POLYPROTEIN

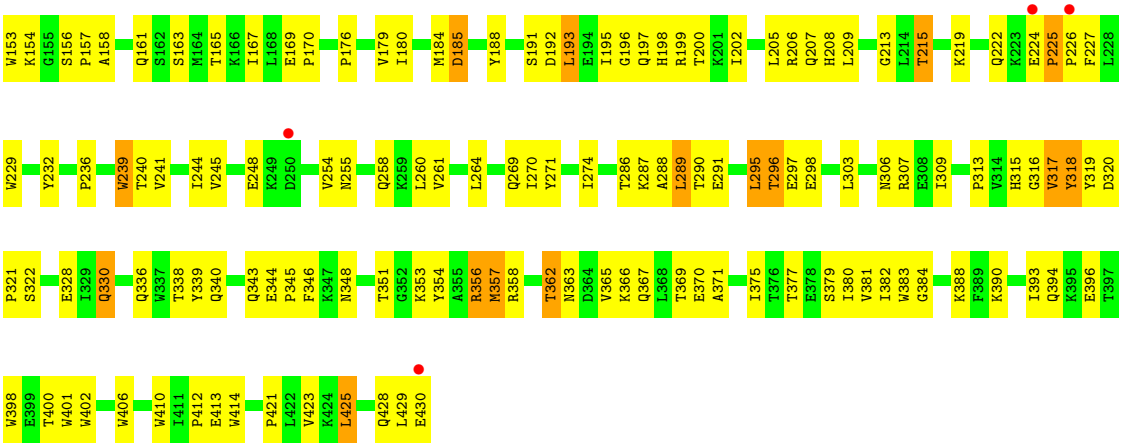
Chain A:



• Molecule 2: POL POLYPROTEIN

Chain B:




W153 K154 G155 S156 P157 A158 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 P176 V179 I180 M184 D185 Y188 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200 K201 I202 L205 R206 Q207 H208 L209 G213 L214 T215 K219 Q222 K223 E224 P225 P226 F227 L228
W229 Y232 P236 W239 T240 V241 I244 V245 E248 K249 D250 V254 N255 Q258 K259 L260 V261 L264 Q269 I270 Y271 I274 T286 K287 A288 L289 T290 E291 L295 T296 E297 E298 L303 M306 R307 E308 I309 P313 V314 H315 G316 V317 Y318 Y319 D320
P321 S322 E328 I329 Q330 Q336 W337 T338 Y339 Q340 Q343 E344 P345 F346 K347 N348 T351 G352 K353 Y354 A355 R356 M357 R358 T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 I375 T376 T377 E378 S379 I380 V381 I382 W383 G384 K388 F389 K390 I393 Q394 K395 E396 T397
W398 E399 T400 W401 W402 W406 W410 I411 P412 E413 W414 P421 L422 V423 K424 L425 Q428 L429 E430

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.10Å 69.00Å 104.00Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 32.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (25.00-3.00) 92.9 (32.75-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.254 , 0.343 0.253 , 0.326	Depositor DCC
R_{free} test set	1480 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 81.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7821	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: AAP

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	0.45	0/4491	0.45	0/6122
2	B	0.51	0/3520	0.49	0/4804
All	All	0.48	0/8011	0.47	0/10926

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	144	TYR	Sidechain

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	4377	0	4280	257	0
2	B	3421	0	3339	192	0
3	A	23	0	16	11	0
All	All	7821	0	7635	441	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 29.

All (441) 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)
2:B:348:ASN:HD22	2:B:351:THR:HG22	1.22	1.04
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.40	0.99
2:B:135:ILE:O	2:B:138:GLU:HG2	1.62	0.99
2:B:255:ASN:HB2	2:B:289:LEU:HD21	1.46	0.94
1:A:195:ILE:HG22	1:A:199:ARG:HH12	1.31	0.94
1:A:460:ASN:H	1:A:460:ASN:HD22	0.95	0.93
1:A:329:ILE:HD13	1:A:391:LEU:HB3	1.51	0.93
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.33	0.89
2:B:289:LEU:HD23	2:B:290:THR:H	1.36	0.89
1:A:54:ASN:N	1:A:55:PRO:HD2	1.88	0.87
1:A:295:LEU:HD12	1:A:295:LEU:H	1.35	0.87
1:A:460:ASN:HD22	1:A:460:ASN:N	1.71	0.87
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.10	0.86
1:A:240:THR:HG22	1:A:241:VAL:H	1.38	0.86
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.11	0.86
1:A:460:ASN:H	1:A:460:ASN:ND2	1.73	0.85
1:A:427:TYR:OH	1:A:509:GLN:HA	1.78	0.83
1:A:195:ILE:HG22	1:A:199:ARG:NH1	1.94	0.82
2:B:31:ILE:O	2:B:35:VAL:HG23	1.80	0.81
2:B:32:LYS:HB2	2:B:32:LYS:HZ2	1.47	0.79
2:B:225:PRO:HB2	2:B:226:PRO:CD	2.13	0.79
1:A:57:ASN:HD21	1:A:131:THR:N	1.81	0.78
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.66	0.78
1:A:408:ALA:O	2:B:393:ILE:HG13	1.83	0.78
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.48	0.78
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.18	0.77
1:A:240:THR:HG22	1:A:241:VAL:N	2.00	0.77
2:B:225:PRO:HB2	2:B:226:PRO:HD3	1.67	0.76
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.67	0.76
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.65	0.75
1:A:181:TYR:CD2	3:A:561:AAP:HM'2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:HB2	1:A:548:VAL:HG12	1.68	0.75
2:B:328:GLU:HB3	2:B:390:LYS:HB2	1.69	0.75
2:B:139:THR:HB	2:B:140:PRO:HD2	1.69	0.74
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.16	0.74
1:A:511:ASP:HA	1:A:522:ILE:HD13	1.69	0.74
1:A:188:TYR:HD2	3:A:561:AAP:CL6	2.06	0.74
2:B:27:THR:HB	2:B:30:LYS:HG3	1.69	0.74
2:B:32:LYS:HB2	2:B:32:LYS:NZ	2.03	0.74
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.23	0.74
1:A:509:GLN:N	1:A:510:PRO:HD3	2.03	0.74
1:A:117:SER:HB2	1:A:214:LEU:HD23	1.70	0.73
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.53	0.73
1:A:89:GLU:HB3	1:A:92:LEU:HB2	1.70	0.72
1:A:57:ASN:HD21	1:A:131:THR:H	1.35	0.72
1:A:17:ASP:O	1:A:83:ARG:HG2	1.90	0.72
2:B:79:GLU:O	2:B:83:ARG:HG2	1.88	0.72
2:B:206:ARG:HH11	2:B:206:ARG:HB3	1.53	0.72
2:B:255:ASN:HB2	2:B:289:LEU:CD2	2.20	0.72
1:A:242:GLN:HB2	1:A:243:PRO:HD3	1.71	0.71
2:B:199:ARG:HH12	2:B:229:TRP:CB	2.04	0.71
1:A:23:GLN:NE2	1:A:60:VAL:H	1.89	0.71
1:A:195:ILE:CG2	1:A:199:ARG:HH12	2.03	0.71
1:A:382:ILE:O	2:B:136:ASN:HB2	1.90	0.71
1:A:461:LYS:HB3	1:A:461:LYS:NZ	2.05	0.71
1:A:395:LYS:O	1:A:399:GLU:HG2	1.90	0.71
2:B:53:GLU:O	2:B:55:PRO:HD3	1.90	0.71
1:A:494:ASN:N	1:A:494:ASN:HD22	1.89	0.70
1:A:59:PRO:O	1:A:75:VAL:HG13	1.91	0.70
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.56	0.70
2:B:356:ARG:NH2	2:B:357:MET:HB3	2.07	0.70
1:A:405:TYR:HE2	1:A:407:GLN:HB3	1.56	0.69
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.75	0.69
1:A:524:GLN:O	1:A:528:LYS:HG2	1.91	0.69
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.01	0.69
2:B:205:LEU:O	2:B:209:LEU:HG	1.92	0.69
1:A:190:GLY:N	3:A:561:AAP:HN2	1.90	0.69
1:A:254:VAL:HB	1:A:289:LEU:HA	1.74	0.69
1:A:329:ILE:HD12	1:A:329:ILE:H	1.58	0.68
2:B:63:ILE:HG22	2:B:64:LYS:N	2.09	0.68
2:B:398:TRP:O	2:B:402:TRP:HD1	1.76	0.68
1:A:257:ILE:O	1:A:261:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ILE:CD1	1:A:391:LEU:HB3	2.24	0.67
1:A:317:VAL:HG22	1:A:318:TYR:H	1.57	0.67
2:B:348:ASN:ND2	2:B:351:THR:HG22	2.03	0.67
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.75	0.67
2:B:224:GLU:HB3	2:B:225:PRO:HD2	1.77	0.67
2:B:261:VAL:HA	2:B:264:LEU:HD12	1.77	0.67
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.30	0.66
1:A:437:ALA:HB3	1:A:494:ASN:HD21	1.60	0.66
1:A:495:ILE:O	1:A:533:LEU:HD12	1.95	0.65
1:A:32:LYS:O	1:A:35:VAL:HG22	1.97	0.65
2:B:63:ILE:HD12	2:B:406:TRP:HB3	1.80	0.64
1:A:440:PHE:O	1:A:442:VAL:HG23	1.97	0.64
1:A:227:PHE:O	1:A:233:GLU:HA	1.97	0.64
2:B:371:ALA:O	2:B:375:ILE:HG12	1.97	0.64
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.13	0.64
1:A:358:ARG:HD2	1:A:358:ARG:N	2.11	0.63
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.46	0.63
1:A:460:ASN:N	1:A:460:ASN:ND2	2.38	0.63
1:A:229:TRP:CD2	1:A:230:MET:HG2	2.33	0.63
1:A:23:GLN:HE22	1:A:60:VAL:H	1.44	0.63
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.13	0.62
1:A:442:VAL:CG1	1:A:481:ALA:HB1	2.29	0.62
1:A:96:HIS:HD1	1:A:98:ALA:H	1.48	0.62
1:A:96:HIS:NE2	1:A:269:GLN:NE2	2.47	0.61
1:A:132:ILE:O	1:A:142:ILE:HD12	2.00	0.61
2:B:64:LYS:HB3	2:B:68:SER:HA	1.82	0.61
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.83	0.61
2:B:224:GLU:HB3	2:B:225:PRO:CD	2.31	0.61
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.63	0.61
2:B:12:LEU:HD12	2:B:12:LEU:H	1.66	0.61
1:A:79:GLU:O	1:A:82:LYS:HB2	2.00	0.61
1:A:131:THR:HG22	1:A:143:ARG:CB	2.31	0.61
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.83	0.60
1:A:301:LEU:O	1:A:305:GLU:HB2	2.02	0.60
2:B:316:GLY:C	2:B:318:TYR:H	2.05	0.60
1:A:419:THR:HG22	1:A:421:PRO:CD	2.24	0.60
1:A:443:ASP:HB2	1:A:548:VAL:CG1	2.32	0.60
1:A:126:LYS:HA	1:A:145:GLN:OE1	2.02	0.59
1:A:46:LYS:HD2	1:A:116:PHE:O	2.02	0.59
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.84	0.59
1:A:54:ASN:N	1:A:55:PRO:CD	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:N	1:A:81:ASN:HD22	2.00	0.59
2:B:236:PRO:HA	2:B:239:TRP:CG	2.38	0.59
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.68	0.59
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.38	0.59
1:A:240:THR:CG2	1:A:241:VAL:H	2.12	0.58
2:B:254:VAL:HG21	2:B:288:ALA:O	2.04	0.58
1:A:366:LYS:O	1:A:370:GLU:HG3	2.04	0.58
1:A:276:VAL:HG12	1:A:276:VAL:O	2.04	0.57
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.38	0.57
1:A:544:GLY:O	1:A:548:VAL:HG23	2.03	0.57
2:B:193:LEU:H	2:B:193:LEU:HD23	1.70	0.57
1:A:20:LYS:HG2	1:A:56:TYR:CB	2.34	0.57
1:A:188:TYR:CE2	3:A:561:AAP:HM51	2.39	0.57
1:A:93:GLY:HA3	2:B:137:ASN:OD1	2.05	0.56
1:A:191:SER:HB3	1:A:198:HIS:HD2	1.70	0.56
1:A:242:GLN:HB2	1:A:243:PRO:CD	2.34	0.56
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.35	0.56
2:B:195:ILE:HG23	2:B:196:GLY:H	1.71	0.56
2:B:366:LYS:O	2:B:370:GLU:HG3	2.05	0.56
1:A:266:TRP:O	1:A:269:GLN:HG3	2.06	0.56
2:B:154:LYS:HG2	2:B:184:MET:SD	2.46	0.56
1:A:191:SER:HB3	1:A:198:HIS:CD2	2.40	0.56
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.20	0.56
1:A:295:LEU:HD12	1:A:295:LEU:N	2.15	0.56
1:A:188:TYR:HB3	3:A:561:AAP:HA	1.88	0.56
1:A:420:PRO:HB2	1:A:421:PRO:CD	2.36	0.56
2:B:29:GLU:HG3	2:B:30:LYS:N	2.21	0.56
1:A:438:GLU:HG2	1:A:460:ASN:HD21	1.71	0.55
2:B:50:ILE:HD11	2:B:144:TYR:O	2.07	0.55
2:B:297:GLU:CG	2:B:298:GLU:H	2.19	0.55
1:A:420:PRO:HB2	1:A:421:PRO:HD3	1.88	0.55
1:A:518:VAL:O	1:A:522:ILE:HG13	2.07	0.55
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.88	0.55
1:A:275:LYS:H	1:A:306:ASN:HD21	1.54	0.55
1:A:240:THR:OG1	1:A:315:HIS:HA	2.07	0.54
2:B:27:THR:O	2:B:31:ILE:HG13	2.08	0.54
1:A:34:LEU:HD13	1:A:132:ILE:HG21	1.90	0.54
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.88	0.54
2:B:49:LYS:HA	2:B:143:ARG:O	2.06	0.54
2:B:142:ILE:H	2:B:142:ILE:HD12	1.71	0.54
1:A:439:THR:H	1:A:460:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ILE:HB	2:B:142:ILE:HD13	1.90	0.54
1:A:398:TRP:O	1:A:401:TRP:HB3	2.07	0.54
2:B:84:THR:OG1	2:B:85:GLN:N	2.40	0.54
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.08	0.54
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.06	0.54
1:A:429:LEU:HD12	1:A:429:LEU:N	2.23	0.54
2:B:56:TYR:HE2	2:B:126:LYS:HE2	1.73	0.54
2:B:339:TYR:CG	2:B:375:ILE:HD12	2.43	0.54
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.73	0.53
2:B:62:ALA:HB1	2:B:71:TRP:CE3	2.44	0.53
1:A:53:GLU:C	1:A:55:PRO:HD2	2.29	0.53
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.91	0.53
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.43	0.53
1:A:254:VAL:HG23	1:A:291:GLU:HG3	1.90	0.53
1:A:357:MET:C	1:A:359:GLY:H	2.12	0.53
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.89	0.52
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.44	0.52
2:B:156:SER:N	2:B:157:PRO:HD2	2.24	0.52
2:B:306:ASN:O	2:B:309:ILE:HG22	2.09	0.52
1:A:390:LYS:HD2	1:A:417:VAL:HG23	1.90	0.52
2:B:63:ILE:CG2	2:B:64:LYS:N	2.72	0.52
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.75	0.52
1:A:205:LEU:O	1:A:208:HIS:HB3	2.10	0.52
1:A:330:GLN:CD	1:A:340:GLN:HE22	2.12	0.52
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.91	0.52
2:B:63:ILE:HG23	2:B:406:TRP:O	2.09	0.52
1:A:114:ALA:HB1	1:A:160:PHE:HE1	1.67	0.52
1:A:125:ARG:NH1	1:A:147:ASN:HD22	2.07	0.52
1:A:329:ILE:HD12	1:A:329:ILE:N	2.24	0.52
2:B:32:LYS:NZ	2:B:32:LYS:CB	2.73	0.52
2:B:65:LYS:H	2:B:72:ARG:HG3	1.74	0.51
2:B:339:TYR:CD2	2:B:375:ILE:HD12	2.44	0.51
2:B:421:PRO:C	2:B:423:VAL:H	2.14	0.51
1:A:520:GLN:O	1:A:524:GLN:HG2	2.10	0.51
2:B:380:ILE:O	2:B:384:GLY:N	2.43	0.51
2:B:158:ALA:O	2:B:161:GLN:HB3	2.10	0.51
1:A:19:PRO:O	1:A:56:TYR:HB2	2.10	0.51
1:A:112:GLY:C	1:A:114:ALA:H	2.14	0.51
2:B:195:ILE:HG23	2:B:196:GLY:N	2.25	0.51
1:A:188:TYR:O	3:A:561:AAP:N	2.43	0.51
2:B:50:ILE:HD12	2:B:143:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG12	1:A:443:ASP:N	2.25	0.51
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.51
1:A:28:GLU:O	1:A:31:ILE:HG22	2.11	0.51
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.40	0.51
2:B:356:ARG:NH2	2:B:357:MET:CB	2.74	0.51
2:B:377:THR:HA	2:B:380:ILE:HG13	1.91	0.51
1:A:23:GLN:OE1	1:A:60:VAL:HG23	2.11	0.50
1:A:116:PHE:O	1:A:148:VAL:HG11	2.11	0.50
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.93	0.50
2:B:13:LYS:HD3	2:B:16:MET:SD	2.51	0.50
2:B:111:VAL:N	2:B:185:ASP:O	2.38	0.50
1:A:253:THR:O	1:A:257:ILE:HG13	2.11	0.50
2:B:351:THR:HB	2:B:429:LEU:HD22	1.92	0.50
2:B:398:TRP:C	2:B:400:THR:H	2.14	0.50
1:A:240:THR:HA	1:A:270:ILE:CD1	2.41	0.50
2:B:44:GLU:C	2:B:46:LYS:H	2.14	0.50
1:A:452:LEU:HD12	1:A:452:LEU:O	2.12	0.49
2:B:303:LEU:O	2:B:307:ARG:HB2	2.12	0.49
1:A:380:ILE:O	1:A:384:GLY:HA2	2.12	0.49
1:A:388:LYS:HD2	1:A:413:GLU:HB3	1.93	0.49
1:A:510:PRO:O	1:A:511:ASP:HB3	2.13	0.49
1:A:295:LEU:H	1:A:295:LEU:CD1	2.12	0.49
1:A:188:TYR:CD1	1:A:188:TYR:N	2.80	0.49
1:A:258:GLN:HE21	1:A:283:LEU:HD21	1.78	0.49
1:A:270:ILE:O	1:A:272:PRO:HD3	2.12	0.49
1:A:377:THR:O	1:A:381:VAL:HG23	2.12	0.49
1:A:433:PRO:HA	1:A:532:TYR:CG	2.47	0.49
1:A:233:GLU:CB	1:A:242:GLN:HG2	2.43	0.49
1:A:255:ASN:HB2	1:A:289:LEU:HB2	1.94	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.93	0.49
1:A:20:LYS:HG2	1:A:56:TYR:HB3	1.95	0.49
1:A:229:TRP:O	1:A:232:TYR:HB2	2.12	0.49
1:A:240:THR:HA	1:A:270:ILE:HD11	1.94	0.49
1:A:106:VAL:HG13	1:A:189:VAL:O	2.13	0.49
2:B:289:LEU:HD23	2:B:290:THR:N	2.17	0.49
2:B:356:ARG:HE	2:B:357:MET:N	2.11	0.49
2:B:295:LEU:HD23	2:B:296:THR:H	1.78	0.49
2:B:44:GLU:O	2:B:46:LYS:N	2.46	0.49
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.95	0.48
1:A:507:GLN:O	1:A:509:GLN:HG3	2.13	0.48
1:A:189:VAL:C	3:A:561:AAP:HN2	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ASP:HA	1:A:552:VAL:HG22	1.95	0.48
1:A:509:GLN:N	1:A:510:PRO:CD	2.76	0.48
2:B:30:LYS:O	2:B:34:LEU:HG	2.14	0.48
2:B:270:ILE:HG13	2:B:346:PHE:HD1	1.79	0.48
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.48	0.48
2:B:12:LEU:HB3	2:B:84:THR:HG22	1.95	0.48
1:A:483:TYR:O	1:A:487:GLN:HG3	2.13	0.48
1:A:317:VAL:HG22	1:A:318:TYR:N	2.28	0.48
1:A:363:ASN:HD21	1:A:425:LEU:HD21	1.79	0.48
1:A:56:TYR:O	1:A:129:ALA:HB3	2.14	0.47
2:B:410:TRP:O	2:B:410:TRP:CE3	2.68	0.47
2:B:109:LEU:O	2:B:109:LEU:HD12	2.14	0.47
1:A:84:THR:HG22	1:A:124:PHE:CZ	2.42	0.47
1:A:240:THR:CG2	1:A:241:VAL:N	2.70	0.47
2:B:12:LEU:HD12	2:B:12:LEU:N	2.28	0.47
2:B:296:THR:HB	2:B:297:GLU:H	1.54	0.47
1:A:329:ILE:HG23	1:A:339:TYR:HB3	1.96	0.47
3:A:561:AAP:CL2	3:A:561:AAP:O	2.70	0.47
2:B:297:GLU:HG3	2:B:298:GLU:H	1.80	0.47
2:B:379:SER:O	2:B:383:TRP:N	2.42	0.47
1:A:188:TYR:CD2	3:A:561:AAP:HM51	2.50	0.46
2:B:344:GLU:HG3	2:B:345:PRO:HD2	1.97	0.46
1:A:89:GLU:CB	1:A:92:LEU:HB2	2.44	0.46
1:A:186:ASP:CB	1:A:188:TYR:HE1	2.16	0.46
2:B:356:ARG:HE	2:B:357:MET:H	1.64	0.46
1:A:225:PRO:CB	1:A:226:PRO:HD3	2.41	0.46
1:A:23:GLN:HE22	1:A:60:VAL:N	2.12	0.46
1:A:188:TYR:C	3:A:561:AAP:HN1	2.19	0.46
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.46	0.46
1:A:218:ASP:HB3	1:A:222:GLN:OE1	2.16	0.45
2:B:94:ILE:HG12	2:B:161:GLN:OE1	2.16	0.45
1:A:117:SER:HB2	1:A:214:LEU:CD2	2.44	0.45
1:A:368:LEU:O	1:A:371:ALA:HB3	2.17	0.45
1:A:8:VAL:CG2	1:A:159:ILE:HG12	2.47	0.45
1:A:341:ILE:O	1:A:349:LEU:HB3	2.16	0.45
2:B:11:LYS:HA	2:B:11:LYS:HD3	1.73	0.45
2:B:81:ASN:OD1	2:B:153:TRP:HD1	1.99	0.45
1:A:57:ASN:HD22	1:A:131:THR:HG23	1.81	0.45
1:A:328:GLU:HA	1:A:390:LYS:O	2.17	0.45
1:A:329:ILE:HD12	1:A:390:LYS:O	2.16	0.45
2:B:49:LYS:CG	2:B:144:TYR:CE1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:GLN:HA	2:B:354:TYR:O	2.16	0.45
1:A:181:TYR:HE1	1:A:183:TYR:HB2	1.79	0.45
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.98	0.45
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.31	0.45
2:B:369:THR:HG22	2:B:370:GLU:N	2.32	0.45
2:B:53:GLU:H	2:B:53:GLU:HG3	1.56	0.44
2:B:78:ARG:NH1	2:B:412:PRO:O	2.50	0.44
1:A:81:ASN:N	1:A:81:ASN:ND2	2.65	0.44
1:A:288:ALA:HB3	1:A:291:GLU:HG2	1.99	0.44
2:B:377:THR:HA	2:B:380:ILE:CG1	2.47	0.44
1:A:159:ILE:O	1:A:162:SER:HB3	2.17	0.44
1:A:387:PRO:HG2	1:A:389:PHE:CE1	2.52	0.44
1:A:461:LYS:HB3	1:A:461:LYS:HZ3	1.77	0.44
1:A:484:LEU:O	1:A:486:LEU:N	2.51	0.44
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.99	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
1:A:438:GLU:CG	1:A:460:ASN:HD21	2.30	0.44
2:B:185:ASP:N	2:B:185:ASP:OD1	2.47	0.44
1:A:182:GLN:HG2	1:A:183:TYR:N	2.33	0.44
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.14	0.44
2:B:356:ARG:CZ	2:B:357:MET:HB3	2.47	0.44
1:A:99:GLY:HA2	1:A:383:TRP:NE1	2.31	0.44
2:B:88:TRP:HA	2:B:91:GLN:HB3	2.00	0.44
2:B:191:SER:OG	2:B:198:HIS:CD2	2.71	0.44
1:A:57:ASN:CG	1:A:58:THR:H	2.20	0.44
1:A:240:THR:HG23	1:A:270:ILE:HD12	2.00	0.44
2:B:49:LYS:HG2	2:B:144:TYR:CE1	2.52	0.44
2:B:56:TYR:CE2	2:B:126:LYS:HE2	2.50	0.44
1:A:117:SER:CB	1:A:214:LEU:HD23	2.44	0.44
1:A:450:THR:OG1	1:A:452:LEU:HG	2.18	0.44
1:A:483:TYR:HA	1:A:486:LEU:HD12	2.00	0.44
2:B:289:LEU:C	2:B:291:GLU:H	2.21	0.44
1:A:57:ASN:ND2	1:A:131:THR:N	2.57	0.44
2:B:318:TYR:CZ	2:B:320:ASP:HB2	2.53	0.44
1:A:95:PRO:HD2	1:A:229:TRP:HH2	1.83	0.43
1:A:120:LEU:N	1:A:147:ASN:O	2.51	0.43
1:A:373:GLN:O	1:A:374:LYS:C	2.55	0.43
1:A:539:HIS:C	1:A:541:GLY:H	2.20	0.43
2:B:213:GLY:C	2:B:215:THR:H	2.20	0.43
2:B:363:ASN:HB3	2:B:366:LYS:HB3	2.00	0.43
1:A:118:VAL:O	1:A:148:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:HD23	2:B:296:THR:N	2.33	0.43
1:A:429:LEU:HD12	1:A:429:LEU:H	1.84	0.43
2:B:29:GLU:HA	2:B:32:LYS:NZ	2.34	0.43
1:A:244:ILE:HG13	1:A:244:ILE:O	2.19	0.43
1:A:274:ILE:HD11	1:A:310:LEU:HD13	2.00	0.43
2:B:222:GLN:CB	2:B:227:PHE:HD1	2.30	0.43
2:B:271:TYR:HB2	2:B:274:ILE:HD11	2.01	0.43
1:A:95:PRO:HA	2:B:136:ASN:O	2.18	0.43
2:B:100:LEU:HG	2:B:381:VAL:HG13	1.99	0.43
2:B:118:VAL:O	2:B:148:VAL:HB	2.18	0.43
2:B:286:THR:HG22	2:B:286:THR:O	2.19	0.43
1:A:201:LYS:O	1:A:204:GLU:HB2	2.17	0.43
1:A:216:THR:HG22	1:A:218:ASP:OD1	2.18	0.43
1:A:406:TRP:CD2	1:A:407:GLN:N	2.86	0.43
2:B:46:LYS:C	2:B:147:ASN:HD22	2.21	0.43
2:B:63:ILE:HG22	2:B:64:LYS:H	1.79	0.43
2:B:120:LEU:HB2	2:B:148:VAL:O	2.17	0.43
1:A:278:GLN:H	1:A:278:GLN:HG2	1.61	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.22	0.43
2:B:388:LYS:HA	2:B:413:GLU:O	2.19	0.43
1:A:135:ILE:C	1:A:137:ASN:H	2.22	0.43
1:A:410:TRP:HB2	2:B:365:VAL:HG23	2.01	0.43
1:A:460:ASN:HB3	2:B:288:ALA:HA	2.00	0.43
2:B:100:LEU:O	2:B:103:ASN:HB2	2.17	0.43
2:B:423:VAL:HG12	2:B:423:VAL:O	2.17	0.43
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.80	0.43
1:A:498:ASP:HB2	1:A:538:ALA:HA	2.00	0.43
2:B:353:LYS:HE2	2:B:353:LYS:HB3	1.84	0.43
1:A:8:VAL:HG21	1:A:159:ILE:HG12	2.01	0.43
1:A:39:THR:HG22	1:A:39:THR:O	2.19	0.43
1:A:46:LYS:CD	1:A:116:PHE:O	2.67	0.43
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.80	0.43
1:A:276:VAL:HG13	1:A:279:LEU:HB3	2.01	0.42
1:A:433:PRO:HD3	2:B:255:ASN:HD22	1.83	0.42
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.33	0.42
1:A:106:VAL:HG12	1:A:107:THR:N	2.34	0.42
1:A:174:GLN:H	1:A:174:GLN:HG2	1.49	0.42
1:A:391:LEU:HD13	1:A:393:ILE:HG22	2.00	0.42
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.01	0.42
2:B:289:LEU:CD2	2:B:290:THR:H	2.19	0.42
1:A:43:LYS:HB3	1:A:43:LYS:HE2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:H	1:A:460:ASN:HD21	1.66	0.42
2:B:63:ILE:CG2	2:B:64:LYS:H	2.32	0.42
1:A:3:SER:HB3	1:A:119:PRO:HD3	2.01	0.42
1:A:120:LEU:HD23	1:A:125:ARG:HD3	2.01	0.42
1:A:485:ALA:O	1:A:489:SER:HB3	2.19	0.42
2:B:65:LYS:O	2:B:66:LYS:C	2.57	0.42
2:B:316:GLY:O	2:B:318:TYR:N	2.51	0.42
1:A:5:ILE:HD12	1:A:6:GLU:OE2	2.20	0.42
1:A:61:PHE:HD1	1:A:61:PHE:HA	1.71	0.42
2:B:142:ILE:HD12	2:B:142:ILE:N	2.34	0.42
1:A:463:ARG:NH2	1:A:488:ASP:O	2.53	0.42
2:B:380:ILE:H	2:B:380:ILE:HG12	1.71	0.42
1:A:171:PHE:C	1:A:173:LYS:H	2.23	0.42
1:A:278:GLN:HE21	1:A:278:GLN:HB3	1.65	0.42
1:A:461:LYS:HB3	1:A:461:LYS:HZ2	1.83	0.42
2:B:202:ILE:HG22	2:B:206:ARG:HD2	2.02	0.42
2:B:316:GLY:C	2:B:318:TYR:N	2.72	0.42
1:A:91:GLN:HG3	1:A:183:TYR:CE1	2.55	0.41
1:A:218:ASP:HB2	1:A:222:GLN:HB2	2.02	0.41
2:B:47:ILE:HG22	2:B:146:TYR:HA	2.02	0.41
2:B:112:GLY:HA3	2:B:185:ASP:HB3	2.02	0.41
1:A:494:ASN:N	1:A:494:ASN:ND2	2.57	0.41
1:A:522:ILE:HA	1:A:525:LEU:HD12	2.03	0.41
2:B:63:ILE:CD1	2:B:406:TRP:HB3	2.49	0.41
2:B:255:ASN:CB	2:B:289:LEU:HD21	2.34	0.41
1:A:188:TYR:N	1:A:188:TYR:HD1	2.18	0.41
1:A:484:LEU:O	1:A:487:GLN:N	2.53	0.41
1:A:488:ASP:N	1:A:488:ASP:OD1	2.53	0.41
1:A:500:GLN:O	1:A:503:LEU:HB3	2.20	0.41
2:B:111:VAL:HG12	2:B:111:VAL:O	2.20	0.41
2:B:410:TRP:O	2:B:410:TRP:HE3	2.02	0.41
1:A:239:TRP:O	1:A:240:THR:OG1	2.34	0.41
2:B:81:ASN:O	2:B:82:LYS:C	2.59	0.41
2:B:101:LYS:HD3	2:B:382:ILE:HG23	2.02	0.41
2:B:199:ARG:O	2:B:202:ILE:HB	2.19	0.41
1:A:103:ASN:HA	1:A:192:ASP:OD1	2.20	0.41
1:A:132:ILE:HG13	1:A:142:ILE:HB	2.01	0.41
1:A:188:TYR:CD2	3:A:561:AAP:H6'	2.55	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.21	0.41
2:B:27:THR:HG22	2:B:28:GLU:N	2.35	0.41
2:B:320:ASP:N	2:B:343:GLN:OE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:PRO:O	2:B:346:PHE:HB2	2.21	0.41
1:A:46:LYS:NZ	1:A:116:PHE:O	2.50	0.41
1:A:160:PHE:O	1:A:161:GLN:C	2.58	0.41
1:A:394:GLN:HE21	1:A:394:GLN:HB3	1.67	0.41
2:B:260:LEU:HG	2:B:264:LEU:HD11	2.03	0.41
2:B:340:GLN:HG2	2:B:430:GLU:N	2.36	0.41
2:B:400:THR:HG22	2:B:401:TRP:CD1	2.56	0.41
1:A:172:LYS:HB2	1:A:172:LYS:HE3	1.80	0.41
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.55	0.41
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.27	0.41
2:B:193:LEU:HD23	2:B:193:LEU:N	2.35	0.41
2:B:344:GLU:HA	2:B:345:PRO:HD3	1.95	0.41
1:A:3:SER:OG	1:A:5:ILE:HG22	2.20	0.41
1:A:42:GLU:HG3	1:A:43:LYS:N	2.35	0.41
1:A:90:VAL:HG22	1:A:158:ALA:HB2	2.03	0.41
1:A:224:GLU:CD	1:A:224:GLU:H	2.23	0.41
1:A:235:HIS:HB3	1:A:236:PRO:HD2	2.03	0.41
1:A:246:LEU:HD21	1:A:310:LEU:CD2	2.51	0.41
1:A:407:GLN:HG3	2:B:393:ILE:HA	2.02	0.41
2:B:196:GLY:O	2:B:200:THR:HG23	2.21	0.41
2:B:396:GLU:H	2:B:396:GLU:CD	2.23	0.41
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.56	0.41
2:B:96:HIS:NE2	2:B:381:VAL:O	2.52	0.41
2:B:421:PRO:C	2:B:423:VAL:N	2.73	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.02	0.40
1:A:255:ASN:HB2	1:A:289:LEU:O	2.21	0.40
2:B:59:PRO:HB2	2:B:76:ASP:CB	2.46	0.40
2:B:356:ARG:HH21	2:B:357:MET:CB	2.34	0.40
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.40
2:B:188:TYR:CD1	2:B:188:TYR:N	2.89	0.40
1:A:319:TYR:CD2	1:A:321:PRO:HD3	2.56	0.40
1:A:493:VAL:HG22	1:A:494:ASN:N	2.36	0.40
2:B:50:ILE:HD11	2:B:144:TYR:C	2.42	0.40
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.22	0.40
2:B:287:LYS:HB3	2:B:287:LYS:NZ	2.37	0.40
1:A:427:TYR:CZ	1:A:509:GLN:HA	2.56	0.40
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.89	0.40
2:B:393:ILE:HG12	2:B:394:GLN:N	2.36	0.40
2:B:126:LYS:HA	2:B:145:GLN:NE2	2.37	0.40
2:B:363:ASN:O	2:B:367:GLN:HG3	2.21	0.40
2:B:425:LEU:HG	2:B:428:GLN:CB	2.52	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	554/560 (99%)	446 (80%)	88 (16%)	20 (4%)	3 19
2	B	428/430 (100%)	332 (78%)	78 (18%)	18 (4%)	3 16
All	All	982/990 (99%)	778 (79%)	166 (17%)	38 (4%)	3 17

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	135	ILE
1	A	361	HIS
1	A	412	PRO
2	B	219	LYS
1	A	85	GLN
1	A	89	GLU
1	A	134	SER
2	B	66	LYS
2	B	92	LEU
2	B	138	GLU
2	B	241	VAL
2	B	315	HIS
2	B	317	VAL
2	B	357	MET
1	A	14	PRO
1	A	195	ILE
1	A	289	LEU
1	A	542	ILE
2	B	45	GLY
2	B	215	THR
2	B	313	PRO

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Mol	Chain	Res	Type
2	B	362	THR
1	A	136	ASN
1	A	540	LYS
2	B	44	GLU
2	B	358	ARG
1	A	90	VAL
1	A	244	ILE
1	A	462	GLY
2	B	244	ILE
2	B	245	VAL
1	A	510	PRO
1	A	274	ILE
2	B	225	PRO
1	A	505	ILE
2	B	176	PRO
1	A	176	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	459/500 (92%)	408 (89%)	51 (11%)	6 25
2	B	360/392 (92%)	327 (91%)	33 (9%)	9 34
All	All	819/892 (92%)	735 (90%)	84 (10%)	7 28

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	53	GLU
1	A	56	TYR
1	A	61	PHE
1	A	73	LYS
1	A	94	ILE
1	A	111	VAL

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Mol	Chain	Res	Type
1	A	121	ASP
1	A	172	LYS
1	A	174	GLN
1	A	175	ASN
1	A	182	GLN
1	A	184	MET
1	A	187	LEU
1	A	188	TYR
1	A	199	ARG
1	A	210	LEU
1	A	224	GLU
1	A	246	LEU
1	A	252	TRP
1	A	263	LYS
1	A	278	GLN
1	A	279	LEU
1	A	282	LEU
1	A	291	GLU
1	A	295	LEU
1	A	306	ASN
1	A	307	ARG
1	A	325	LEU
1	A	329	ILE
1	A	330	GLN
1	A	334	GLN
1	A	348	ASN
1	A	350	LYS
1	A	353	LYS
1	A	357	MET
1	A	358	ARG
1	A	391	LEU
1	A	402	TRP
1	A	409	THR
1	A	431	LYS
1	A	443	ASP
1	A	460	ASN
1	A	461	LYS
1	A	463	ARG
1	A	488	ASP
1	A	494	ASN
1	A	497	THR
1	A	540	LYS

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Mol	Chain	Res	Type
1	A	546	GLU
1	A	547	GLN
2	B	12	LEU
2	B	50	ILE
2	B	53	GLU
2	B	67	ASP
2	B	87	PHE
2	B	113	ASP
2	B	115	TYR
2	B	123	ASP
2	B	151	GLN
2	B	165	THR
2	B	169	GLU
2	B	179	VAL
2	B	180	ILE
2	B	185	ASP
2	B	193	LEU
2	B	197	GLN
2	B	207	GLN
2	B	232	TYR
2	B	239	TRP
2	B	240	THR
2	B	248	GLU
2	B	269	GLN
2	B	289	LEU
2	B	295	LEU
2	B	296	THR
2	B	317	VAL
2	B	318	TYR
2	B	322	SER
2	B	330	GLN
2	B	356	ARG
2	B	362	THR
2	B	414	TRP
2	B	425	LEU

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	81	ASN
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	197	GLN
1	A	258	GLN
1	A	269	GLN
1	A	278	GLN
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	373	GLN
1	A	394	GLN
1	A	460	ASN
1	A	494	ASN
1	A	519	ASN
1	A	545	ASN
2	B	57	ASN
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	198	HIS
2	B	255	ASN
2	B	258	GLN
2	B	269	GLN
2	B	332	GLN
2	B	348	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AAP	A	561	-	24,24,24	3.15	11 (45%)	27,34,34	1.08	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AAP	A	561	-	-	0/16/16/16	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	AAP	C6'-C1'	6.53	1.49	1.39
3	A	561	AAP	C2-C1	6.31	1.48	1.39
3	A	561	AAP	C6-CL6	6.02	1.87	1.73
3	A	561	AAP	C2-CL2	5.46	1.86	1.73
3	A	561	AAP	C3'-C2'	4.49	1.47	1.39
3	A	561	AAP	C6'-C5'	4.06	1.45	1.39
3	A	561	AAP	C1'-N'	3.59	1.45	1.37
3	A	561	AAP	C2'-C1'	2.77	1.45	1.41
3	A	561	AAP	O'-C'	2.72	1.31	1.22
3	A	561	AAP	C1-CA	2.46	1.58	1.52
3	A	561	AAP	C2'-C'	2.04	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	561	AAP	O'-C'-C2'	2.18	123.44	120.56
3	A	561	AAP	C1-C2-CL2	2.06	122.48	120.49

There are no chirality outliers.

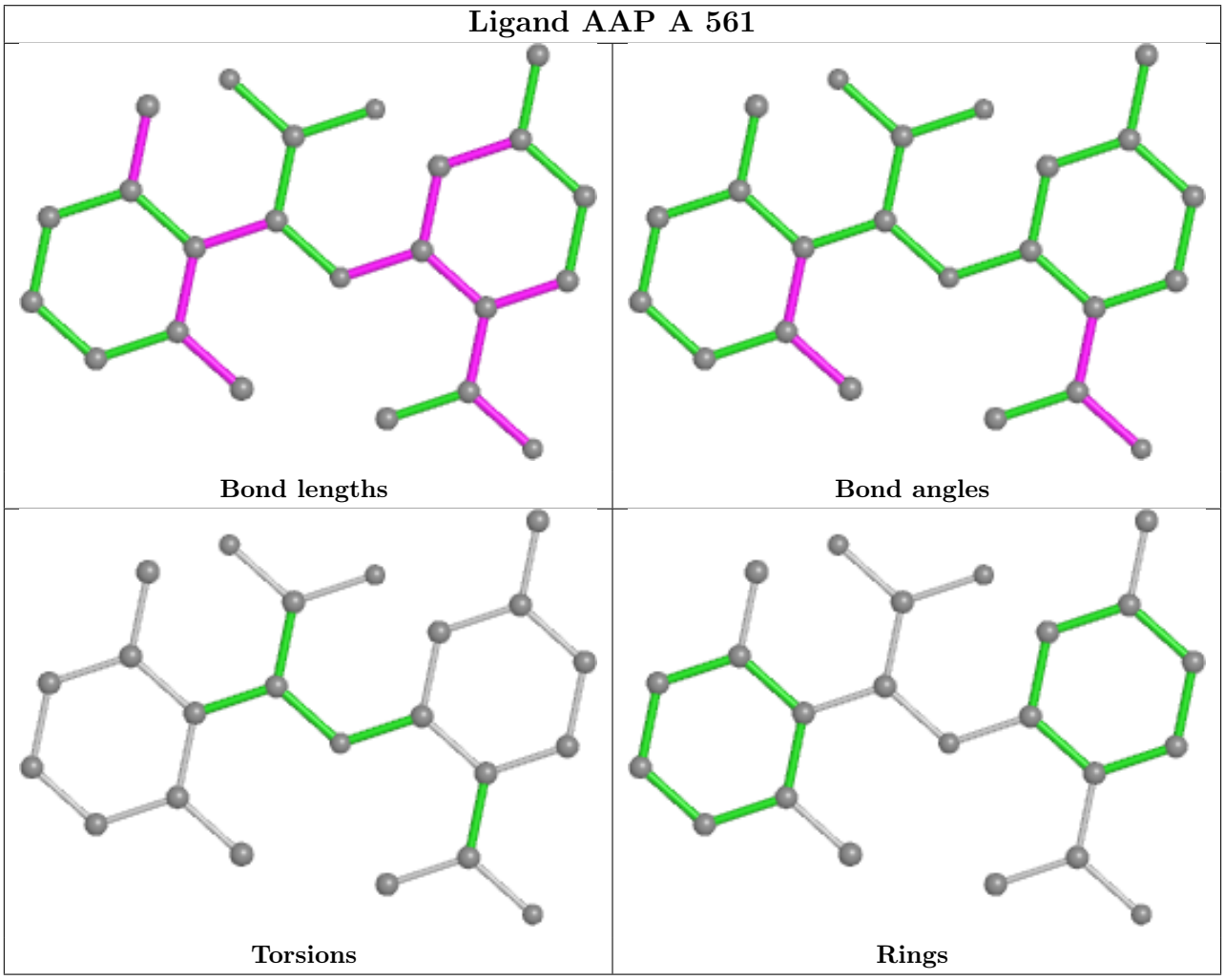
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	AAP	11	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.



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	556/560 (99%)	-0.32	10 (1%) 68 40	12, 72, 100, 100	0
2	B	430/430 (100%)	-0.39	8 (1%) 66 37	8, 57, 100, 100	0
All	All	986/990 (99%)	-0.35	18 (1%) 68 40	8, 68, 100, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	SER	6.5
2	B	1	PRO	4.7
1	A	217	PRO	4.1
1	A	553	SER	4.1
1	A	141	GLY	3.8
1	A	133	PRO	3.7
1	A	554	ALA	3.3
2	B	226	PRO	3.3
2	B	4	PRO	3.2
1	A	221	HIS	3.2
2	B	2	ILE	3.1
1	A	551	LEU	2.7
2	B	430	GLU	2.7
1	A	68	SER	2.7
1	A	222	GLN	2.4
2	B	250	ASP	2.3
1	A	420	PRO	2.2
2	B	224	GLU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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)

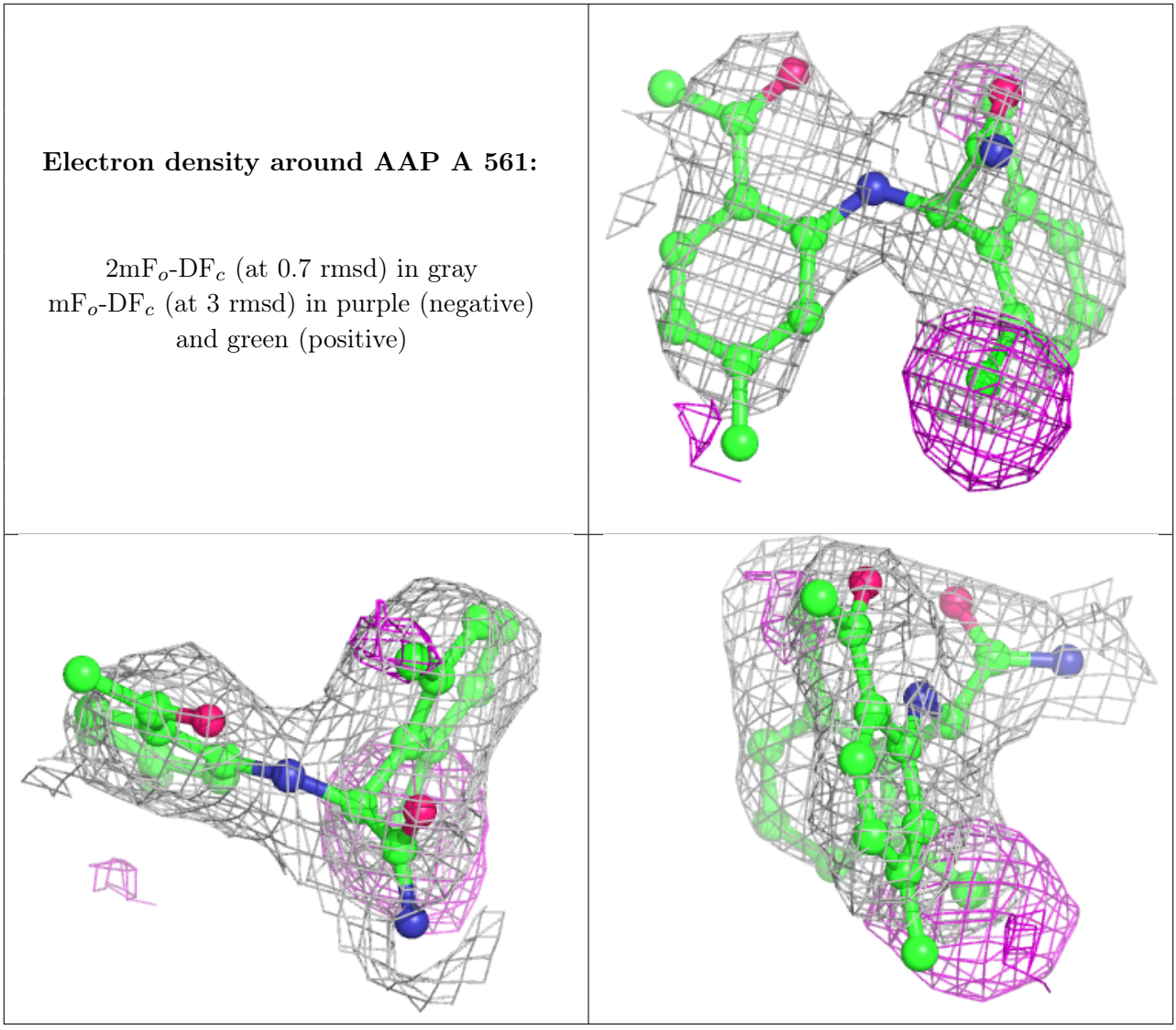
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	AAP	A	561	23/23	0.85	0.28	24,67,86,91	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 AAP A 561:

$2mF_o$-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.