



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:05 AM UTC

PDB ID : 1HPZ / pdb_00001hpz
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

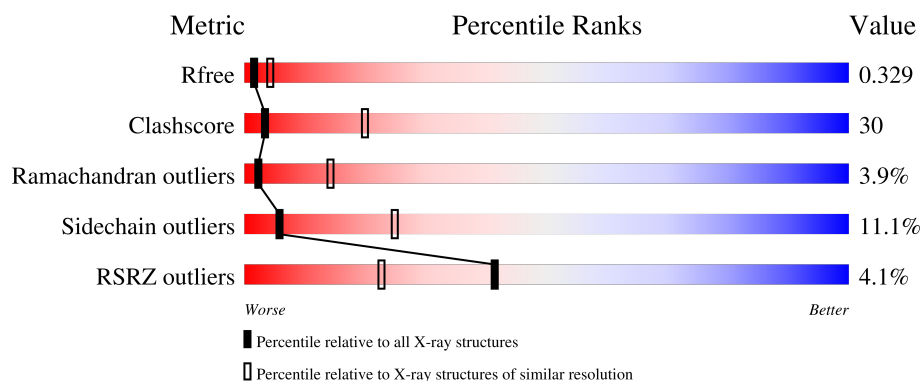
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	430	

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

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

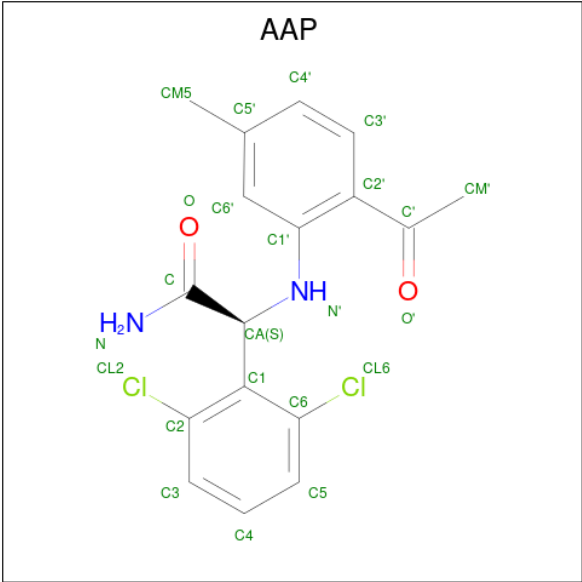
- Molecule 2 is a protein called POL POLYPROTEIN.

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 (CCD ID: AAP) (formula: C₁₇H₁₆Cl₂N₂O₂).

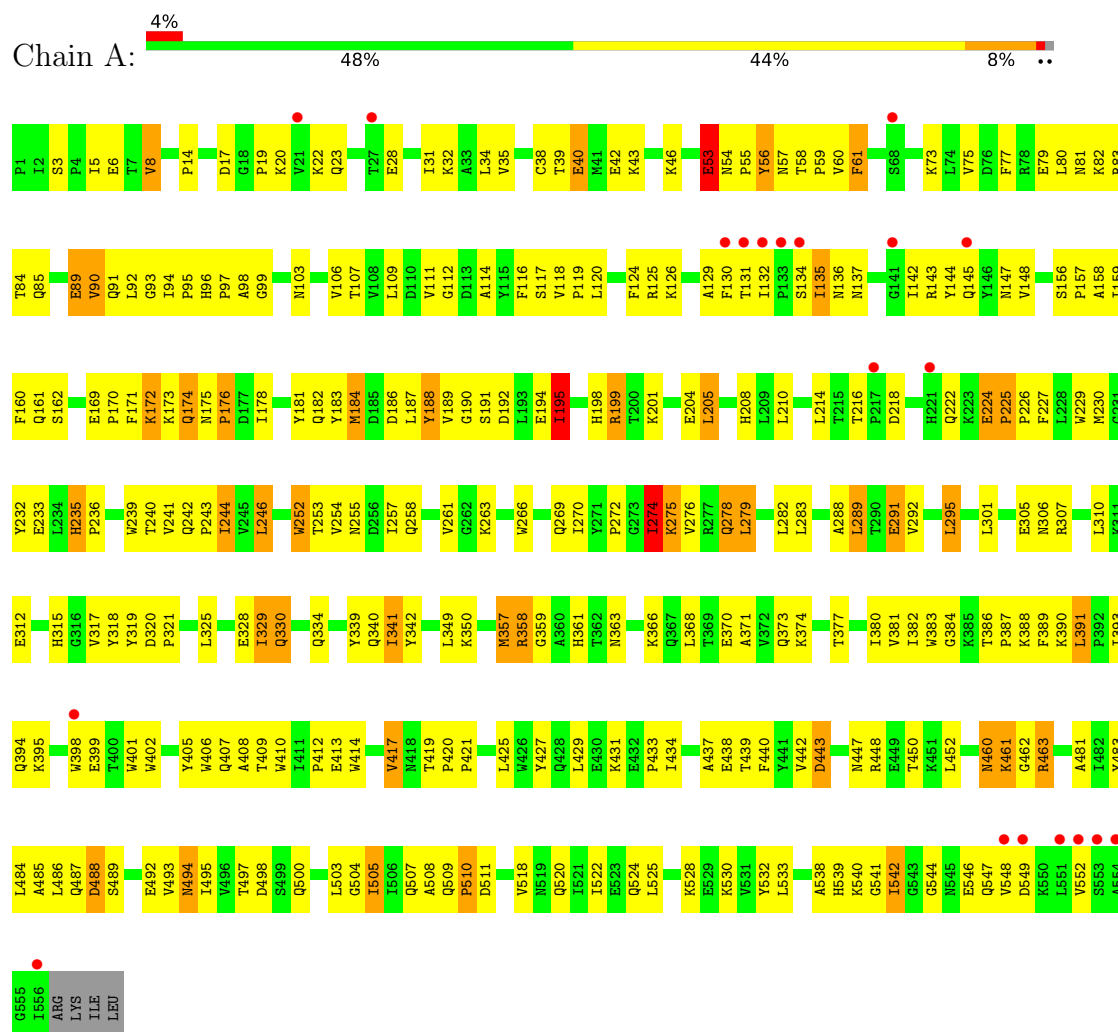


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	23	17	2	2	2	0	0

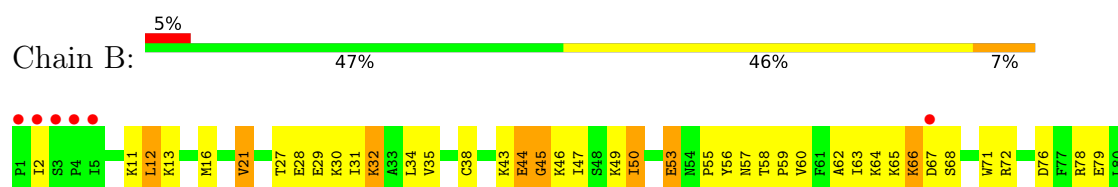
3 Residue-property plots

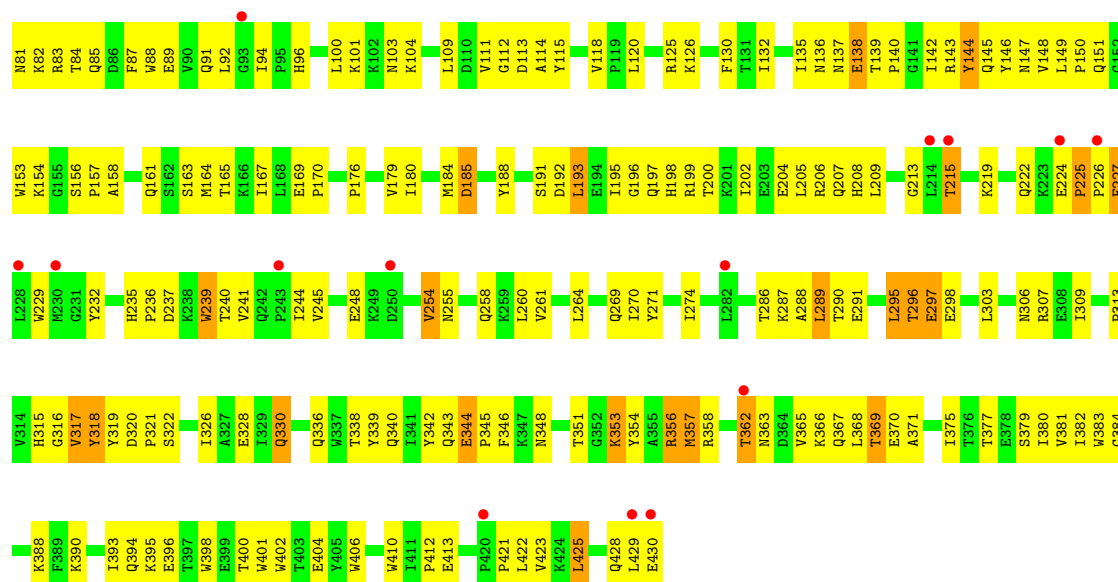
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 2: POL POLYPROTEIN





4 Data and refinement statistics

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 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.8 (25.00-3.00) 92.7 (25.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.254 , 0.343 0.254 , 0.329	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)	0.26 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/4491	0.83	10/6122 (0.2%)
2	B	0.64	1/3520 (0.0%)	0.85	5/4804 (0.1%)
All	All	0.60	1/8011 (0.0%)	0.84	15/10926 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	ILE	CA-CB	5.22	1.59	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	CA-C-N	6.42	126.37	119.76
1	A	312	GLU	C-N-CA	6.42	126.37	119.76
1	A	224	GLU	CA-C-N	6.40	126.97	120.38
1	A	224	GLU	C-N-CA	6.40	126.97	120.38
2	B	227	PHE	N-CA-C	6.32	119.78	110.30
2	B	89	GLU	N-CA-C	-6.21	105.53	113.23
1	A	386	THR	CA-C-N	5.73	125.93	120.31
1	A	386	THR	C-N-CA	5.73	125.93	120.31
2	B	344	GLU	CA-C-N	5.50	126.72	119.84
2	B	344	GLU	C-N-CA	5.50	126.72	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	VAL	CA-C-N	5.41	125.58	119.90
1	A	8	VAL	C-N-CA	5.41	125.58	119.90
2	B	422	LEU	N-CA-C	-5.14	107.08	113.19
1	A	235	HIS	CA-C-N	5.08	126.19	119.84
1	A	235	HIS	C-N-CA	5.08	126.19	119.84

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	268	0
2	B	3421	0	3339	206	0
3	A	23	0	16	11	0
All	All	7821	0	7635	466	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 30.

All (466) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:316:GLY:C	2:B:318:TYR:H	2.05	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:111:VAL:HG11	2:B:164:MET:HE1	1.81	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
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
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:53:GLU:C	1:A:55:PRO:HD2	2.29	0.57
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:357:MET:C	1:A:359:GLY:H	2.12	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:330:GLN:CD	1:A:340:GLN:HE22	2.12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:421:PRO:C	2:B:423:VAL:H	2.14	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:112:GLY:C	1:A:114:ALA:H	2.14	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
2:B:44:GLU:C	2:B:46:LYS:H	2.14	0.54
1:A:34:LEU:HD13	1:A:132:ILE:HG21	1.90	0.54
2:B:398:TRP:C	2:B:400:THR:H	2.14	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
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:189:VAL:C	3:A:561:AAP:HN2	2.17	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:461:LYS:HB3	1:A:461:LYS:HZ3	1.74	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: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
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
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
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:188:TYR:C	3:A:561:AAP:HN1	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HA	1:A:270:ILE:CD1	2.41	0.50
2:B:213:GLY:C	2:B:215:THR:H	2.20	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: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
1:A:510:PRO:O	1:A:511:ASP:HB3	2.13	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
1:A:252:TRP:CD1	1:A:252:TRP:H	2.31	0.49
2:B:289:LEU:C	2:B:291:GLU:H	2.21	0.49
2:B:295:LEU:HD23	2:B:296:THR:H	1.78	0.49
1:A:57:ASN:CG	1:A:58:THR:H	2.20	0.49
2:B:44:GLU:O	2:B:46:LYS:N	2.46	0.49
1:A:539:HIS:C	1:A:541:GLY:H	2.20	0.48
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.95	0.48
1:A:373:GLN:O	1:A:374:LYS:C	2.55	0.48
1:A:507:GLN:O	1:A:509:GLN:HG3	2.13	0.48
1:A:549:ASP:HA	1:A:552:VAL:HG22	1.95	0.48
2:B:153:TRP:CD1	2:B:154:LYS:H	2.32	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
2:B:184:MET:HE2	2:B:410:TRP:HB3	1.96	0.48
1:A:317:VAL:HG22	1:A:318:TYR:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HD21	1:A:425:LEU:HD21	1.79	0.48
2:B:43:LYS:C	2:B:45:GLY:H	2.22	0.48
1:A:135:ILE:C	1:A:137:ASN:H	2.22	0.47
2:B:46:LYS:C	2:B:147:ASN:HD22	2.21	0.47
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
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:65:LYS:O	2:B:66:LYS:C	2.57	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
2:B:396:GLU:CD	2:B:396:GLU:H	2.23	0.46
1:A:171:PHE:C	1:A:173:LYS:H	2.23	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
2:B:81:ASN:O	2:B:82:LYS:C	2.59	0.46
2:B:316:GLY:C	2:B:318:TYR:N	2.72	0.46
1:A:23:GLN:HE22	1:A:60:VAL:N	2.12	0.46
1:A:160:PHE:O	1:A:161:GLN:C	2.58	0.46
2:B:421:PRO:C	2:B:423:VAL:N	2.73	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:224:GLU:CD	1:A:224:GLU:H	2.23	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:427:TYR:HH	1:A:509:GLN:HA	1.78	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:50:ILE:HD11	2:B:144:TYR:C	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:379:SER:O	2:B:380:ILE:C	2.61	0.44
2:B:398:TRP:C	2:B:400:THR:N	2.74	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
2:B:342:TYR:CD1	2:B:342:TYR:C	2.96	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
1:A:57:ASN:ND2	1:A:131:THR:N	2.57	0.44
2:B:112:GLY:C	2:B:114:ALA:H	2.26	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
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

Continued on next page...

Continued from previous page...

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: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
2:B:356:ARG:O	2:B:357:MET:C	2.61	0.43
1:A:278:GLN:H	1:A:278:GLN:HG2	1.61	0.43
2:B:388:LYS:HA	2:B:413:GLU:O	2.19	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: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
2:B:235:HIS:C	2:B:237:ASP:H	2.27	0.42
2:B:365:VAL:O	2:B:366:LYS:C	2.62	0.42
1:A:106:VAL:HG12	1:A:107:THR:N	2.34	0.42
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.01	0.42
1:A:188:TYR:C	3:A:561:AAP:N	2.77	0.42
2:B:289:LEU:CD2	2:B:290:THR:H	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:C	1:A:40:GLU:H	2.28	0.42
1:A:43:LYS:HB3	1:A:43:LYS:HE2	1.89	0.42
1:A:439:THR:H	1:A:460:ASN:HD21	1.66	0.42
2:B:57:ASN:CG	2:B:58:THR:H	2.28	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:316:GLY:O	2:B:318:TYR:N	2.51	0.42
2:B:367:GLN:O	2:B:368:LEU:C	2.62	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
1:A:189:VAL:C	3:A:561:AAP:N	2.77	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
1:A:504:GLY:O	1:A:505:ILE:C	2.62	0.42
2:B:380:ILE:H	2:B:380:ILE:HG12	1.71	0.42
1:A:176:PRO:C	1:A:178:ILE:H	2.27	0.42
1:A:278:GLN:HE21	1:A:278:GLN:HB3	1.65	0.42
1:A:508:ALA:C	1:A:510:PRO:HD3	2.45	0.42
2:B:202:ILE:HG22	2:B:206:ARG:HD2	2.02	0.42
2:B:402:TRP:C	2:B:404:GLU:H	2.28	0.42
1:A:91:GLN:HG3	1:A:183:TYR:CE1	2.55	0.41
1:A:194:GLU:O	1:A:195:ILE:C	2.62	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:345:PRO:O	2:B:346:PHE:HB2	2.21	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
1:A:447:ASN:O	1:A:448:ARG:C	2.63	0.41
1:A:484:LEU:O	1:A:485:ALA:C	2.64	0.41
1:A:542:ILE:C	1:A:544:GLY:H	2.27	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:90:VAL:HG22	1:A:158:ALA:HB2	2.03	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
1:A:159:ILE:O	1:A:160:PHE:C	2.63	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
1:A:112:GLY:C	1:A:114:ALA:N	2.79	0.40
1:A:201:LYS:HD3	1:A:204:GLU:CD	2.46	0.40
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:161:GLN:C	1:A:161:GLN:CD	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: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
2:B:394:GLN:O	2:B:395:LYS:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HG3	1:A:43:LYS:N	2.35	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%)	2	16
2	B	428/430 (100%)	332 (78%)	78 (18%)	18 (4%)	2	13
All	All	982/990 (99%)	778 (79%)	166 (17%)	38 (4%)	2	14

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 ⓘ

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%)	407 (89%)	52 (11%)	5	24
2	B	360/392 (92%)	321 (89%)	39 (11%)	6	26
All	All	819/892 (92%)	728 (89%)	91 (11%)	6	25

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	40	GLU
1	A	53	GLU
1	A	56	TYR
1	A	61	PHE
1	A	73	LYS
1	A	94	ILE
1	A	111	VAL
1	A	172	LYS
1	A	174	GLN
1	A	175	ASN
1	A	184	MET
1	A	187	LEU
1	A	188	TYR
1	A	195	ILE
1	A	199	ARG
1	A	205	LEU
1	A	210	LEU
1	A	225	PRO
1	A	246	LEU
1	A	252	TRP
1	A	263	LYS
1	A	274	ILE
1	A	275	LYS
1	A	278	GLN
1	A	279	LEU
1	A	282	LEU
1	A	291	GLU
1	A	295	LEU
1	A	307	ARG
1	A	325	LEU
1	A	329	ILE
1	A	330	GLN
1	A	334	GLN
1	A	341	ILE
1	A	350	LYS
1	A	357	MET
1	A	358	ARG
1	A	391	LEU
1	A	402	TRP
1	A	409	THR
1	A	417	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	546	GLU
1	A	547	GLN
2	B	12	LEU
2	B	21	VAL
2	B	32	LYS
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	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	204	GLU
2	B	207	GLN
2	B	232	TYR
2	B	239	TRP
2	B	240	THR
2	B	248	GLU
2	B	254	VAL
2	B	269	GLN
2	B	289	LEU
2	B	295	LEU
2	B	296	THR
2	B	297	GLU
2	B	317	VAL
2	B	318	TYR
2	B	322	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	326	ILE
2	B	330	GLN
2	B	353	LYS
2	B	356	ARG
2	B	362	THR
2	B	369	THR
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ASN
1	A	81	ASN
1	A	103	ASN
1	A	147	ASN
1	A	197	GLN
1	A	198	HIS
1	A	255	ASN
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	394	GLN
1	A	460	ASN
1	A	494	ASN
1	A	509	GLN
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	207	GLN
2	B	255	ASN
2	B	258	GLN
2	B	265	ASN
2	B	269	GLN
2	B	330	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 oligosaccharides 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	-	23,24,24	3.26	10 (43%)	30,34,34	1.12	1 (3%)

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	-	-	2/16/16/16	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	AAP	C2-C1	6.51	1.48	1.39
3	A	561	AAP	C6'-C1'	6.45	1.49	1.39
3	A	561	AAP	C6-CL6	6.04	1.87	1.73
3	A	561	AAP	C2-CL2	5.49	1.86	1.73
3	A	561	AAP	C3'-C2'	4.69	1.47	1.39
3	A	561	AAP	C6'-C5'	4.35	1.45	1.39
3	A	561	AAP	C1'-N'	3.76	1.45	1.37
3	A	561	AAP	O'-C'	2.89	1.31	1.22
3	A	561	AAP	C2'-C1'	2.79	1.45	1.41
3	A	561	AAP	C2'-C'	2.02	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	AAP	O'-C'-C2'	2.07	123.44	120.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

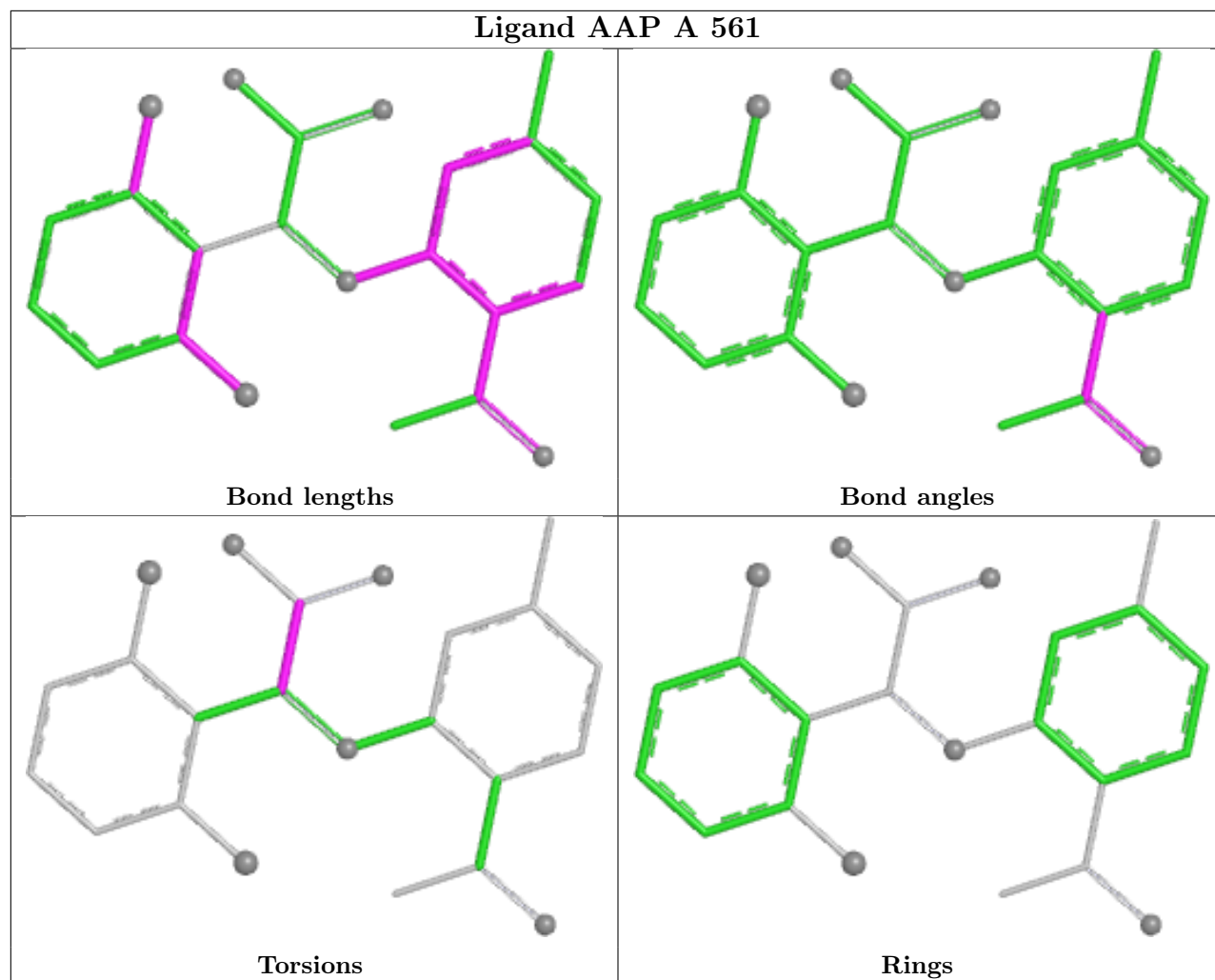
Mol	Chain	Res	Type	Atoms
3	A	561	AAP	O-C-CA-C1
3	A	561	AAP	N-C-CA-C1

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	556/560 (99%)	0.34	20 (3%) 46 26	12, 72, 100, 100	0
2	B	430/430 (100%)	0.13	20 (4%) 36 19	8, 57, 100, 100	0
All	All	986/990 (99%)	0.25	40 (4%) 41 23	8, 68, 100, 100	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	SER	7.3
1	A	551	LEU	4.3
2	B	2	ILE	4.1
1	A	133	PRO	4.0
2	B	226	PRO	3.6
1	A	221	HIS	3.4
2	B	1	PRO	3.3
2	B	430	GLU	3.3
2	B	420	PRO	3.3
1	A	217	PRO	3.2
2	B	4	PRO	3.1
1	A	552	VAL	3.0
1	A	554	ALA	2.9
1	A	548	VAL	2.9
1	A	556	ILE	2.8
2	B	224	GLU	2.8
2	B	214	LEU	2.8
1	A	68	SER	2.7
1	A	141	GLY	2.7
2	B	5	ILE	2.6
1	A	131	THR	2.6
1	A	21	VAL	2.5
1	A	27	THR	2.4
2	B	250	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	429	LEU	2.3
2	B	67	ASP	2.3
2	B	228	LEU	2.3
2	B	215	THR	2.3
2	B	243	PRO	2.3
1	A	553	SER	2.3
1	A	549	ASP	2.2
1	A	398	TRP	2.2
1	A	134	SER	2.2
1	A	145	GLN	2.2
2	B	230	MET	2.2
1	A	130	PHE	2.1
2	B	362	THR	2.1
2	B	93	GLY	2.1
1	A	132	ILE	2.0
2	B	282	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

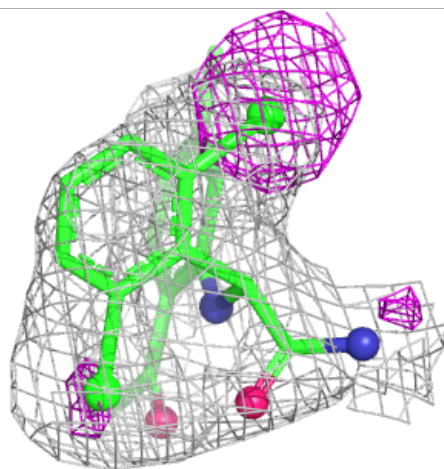
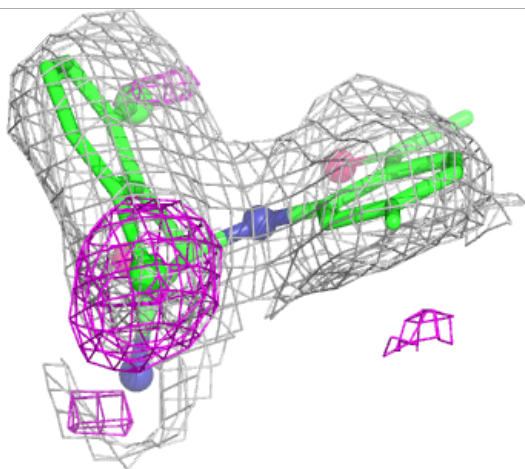
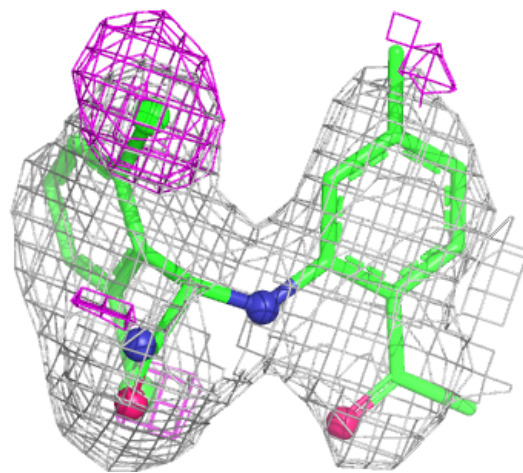
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AAP	A	561	23/23	0.85	0.17	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.