



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:51 PM UTC

PDB ID : 8U6H / pdb_00008u6h
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with 3-(2-(2-(3-acryloyl-2-oxo-2,3-dihydro-1H-benzo[d]imidazol-1-yl)ethoxy)-4-chlorophenoxy)-5-chlorobenzonitrile (JLJ744), a non-nucleoside inhibitor
Authors : Prucha, G.; Carter, Z.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-09-13
Resolution : 2.99 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

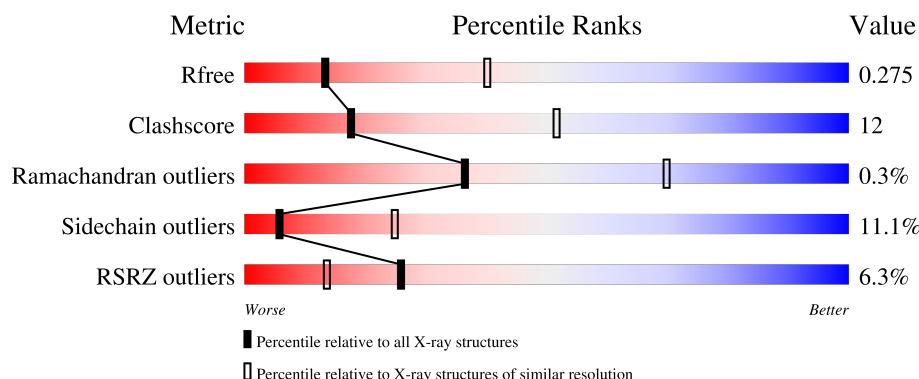
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	556	4% 68% 26% • •
1	C	556	10% 68% 25% • •
2	B	428	2% 67% 24% • 6%
2	D	428	8% 68% 20% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14102 atoms, of which 17 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4192	2701	698	787	6			
1	C	531	Total	C	N	O	S	0	1	0
			3794	2418	645	727	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	172	ALA	LYS	engineered mutation	UNP P03366
C	173	ALA	LYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3230	2097	527	601	5			
2	D	395	Total	C	N	O	S	2	1	0
			2774	1775	472	524	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

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- ORTEP diagram of the chemical structure of 2,2-bis[4-chlorophenyl]-4,4'-nitro-1,1'-biphenyl-5,5'-dicarbonyl. The structure shows two 4-chlorophenyl rings connected by a biphenyl core. The biphenyl core has nitro groups at the 4 and 4' positions and carbonyl groups at the 2 and 2' positions. The carbonyl groups are further substituted with a 2-chloroethyl group and a 2-nitroethyl group. The structure is shown with thermal ellipsoids at the 50% probability level.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 34	C 25	Cl 2	N 3	O 4	0	0
3	C	1	Total 51	C 25	Cl 2	H 17	N 3	O 4	0

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- Diagram illustrating the structure of a phosphate group (PO₄). The central phosphorus atom (P) is bonded to four oxygen atoms (O). The top oxygen is labeled O₃, the bottom O₄, the left O₂, and the right O₁. The central phosphorus is labeled P. The top oxygen has a negative charge (O⁻).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

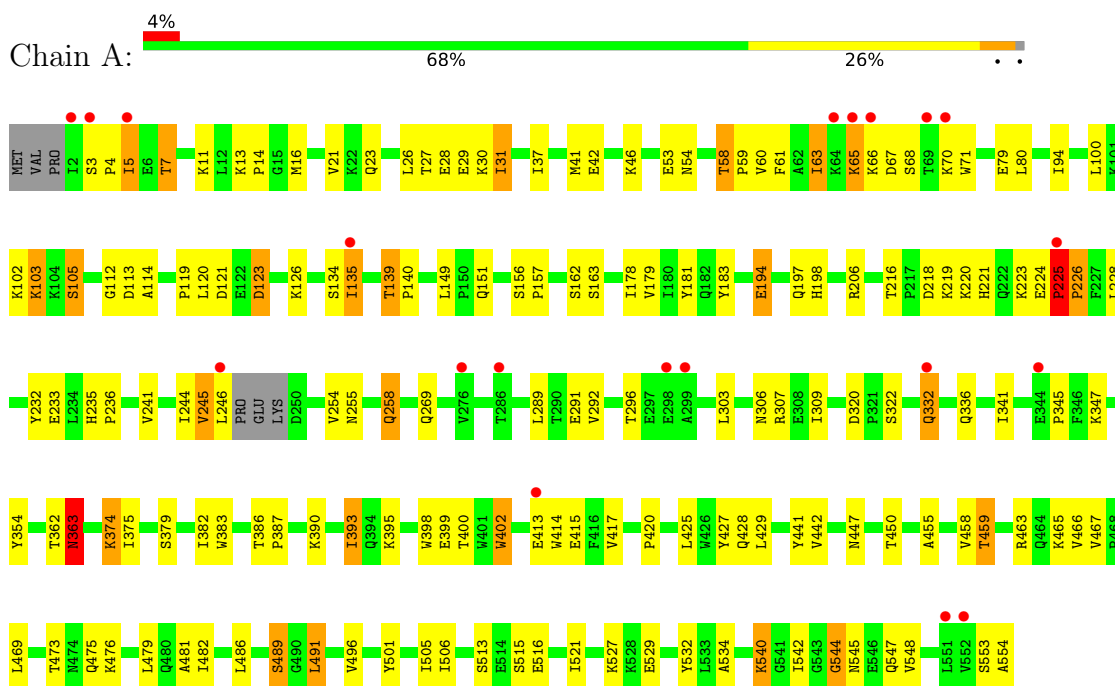
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	6	Total	O	0	0
			6	6		
5	C	2	Total	O	0	0
			2	2		

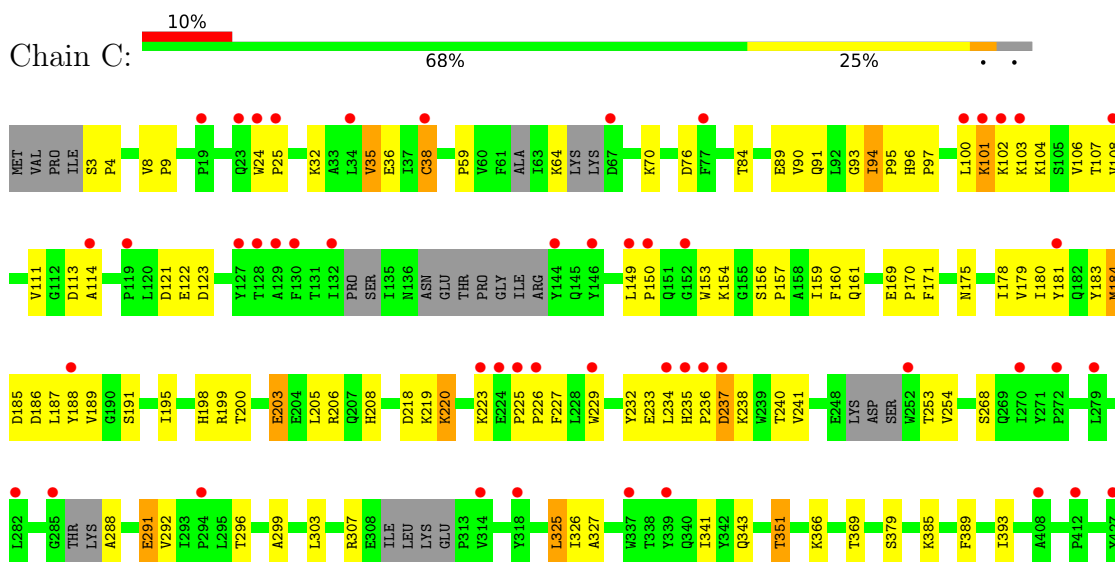
3 Residue-property plots

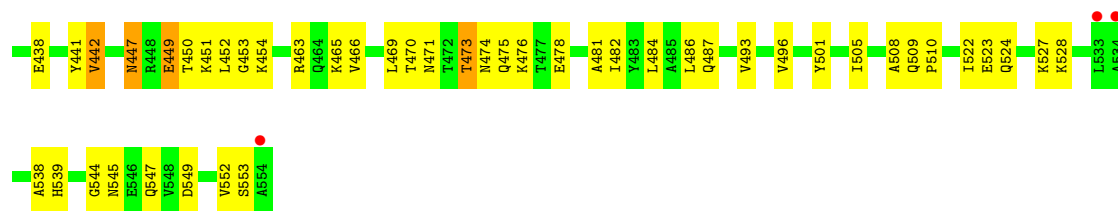
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

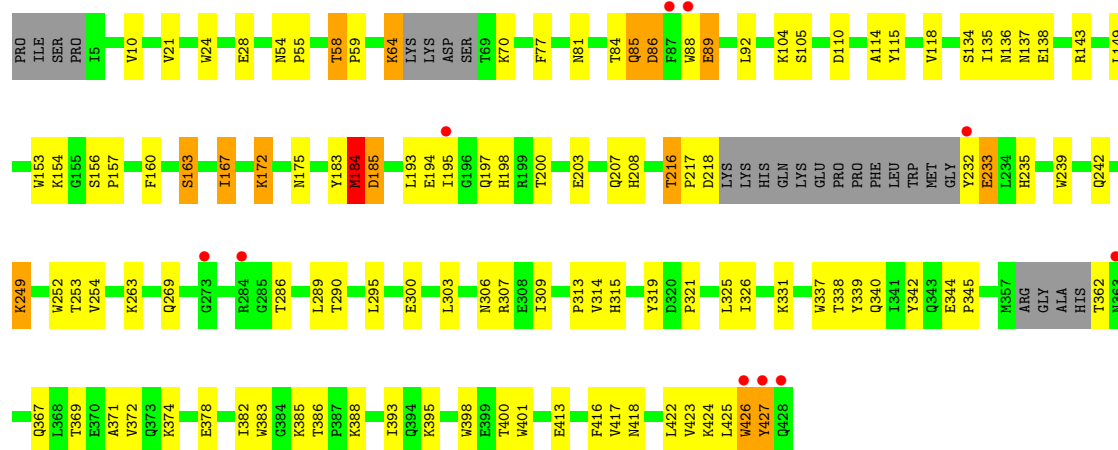


• Molecule 1: Reverse transcriptase/ribonuclease H

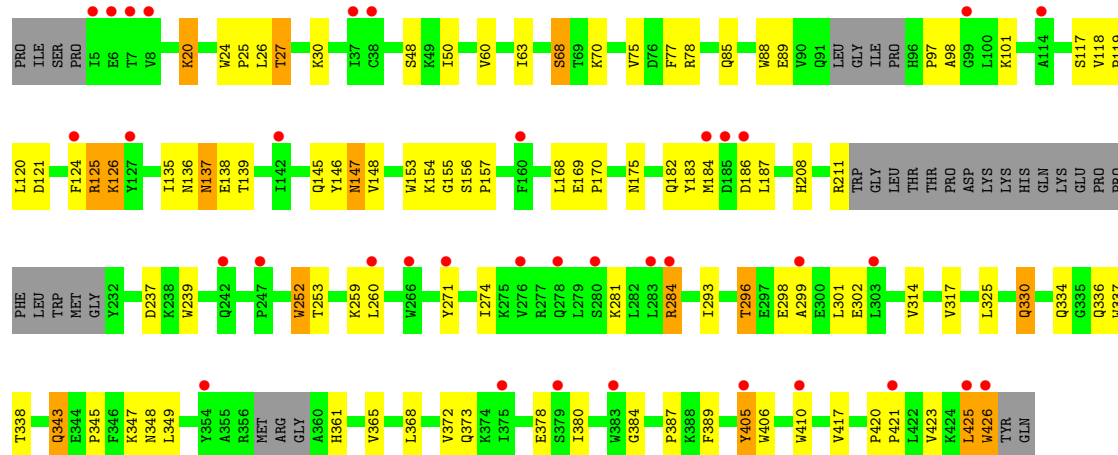




• Molecule 2: p51 RT



• Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.40Å 73.19Å 171.58Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	170.11 – 2.99 170.11 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (170.11-2.99) 99.5 (170.11-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.220 , 0.279 0.263 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 92.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14102	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PO4, VVE

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	0.71	0/4303	1.16	11/5889 (0.2%)
1	C	0.69	0/3892	1.03	1/5346 (0.0%)
2	B	0.68	0/3322	1.16	3/4538 (0.1%)
2	D	0.71	0/2851	1.11	5/3940 (0.1%)
All	All	0.70	0/14368	1.12	20/19713 (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	D	0	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	349	LEU	N-CA-C	-10.71	100.34	113.41
1	A	67	ASP	N-CA-C	-10.36	100.25	113.72
1	A	544	GLY	N-CA-C	-10.30	99.59	112.77
2	D	348	ASN	N-CA-C	-7.81	98.32	109.96
2	D	348	ASN	CB-CA-C	7.47	120.92	110.16
1	A	4	PRO	N-CA-C	-7.30	107.09	114.68
1	A	58	THR	CB-CA-C	7.06	119.50	108.84
1	C	343	GLN	N-CA-C	-6.08	105.89	113.55
1	A	220	LYS	N-CA-C	-5.88	104.77	112.41
2	B	269	GLN	CB-CA-C	5.76	119.88	110.95
2	D	343	GLN	N-CA-C	-5.74	106.41	113.41
1	A	66	LYS	N-CA-C	5.62	117.58	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PRO	N-CA-C	5.54	120.85	114.03
2	D	271	TYR	N-CA-C	-5.49	101.29	109.42
1	A	59	PRO	CB-CA-C	-5.47	103.81	110.98
1	A	347	LYS	CB-CA-C	5.18	120.21	111.41
2	B	137	ASN	CB-CA-C	-5.14	104.29	111.80
1	A	363	ASN	CB-CA-C	5.13	117.99	109.72
1	A	420	PRO	N-CA-CB	5.04	106.01	103.19
2	B	59	PRO	N-CA-C	5.04	119.14	111.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	97	PRO	Mainchain
2	D	98[A]	ALA	Mainchain
2	D	98[B]	ALA	Mainchain

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	4192	0	3936	97	0
1	C	3794	0	3243	112	0
2	B	3230	0	3113	67	0
2	D	2774	0	2275	60	0
3	A	34	0	0	8	0
3	C	34	17	0	6	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	9	0	0	0	0
5	B	6	0	0	0	0
5	C	2	0	0	0	0
All	All	14085	17	12567	329	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 12.

All (329) 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:D:182:GLN:HA	2:D:187:LEU:HA	1.36	1.07
3:C:601:VVE:C1	3:C:601:VVE:O2	2.17	0.92
1:A:102:LYS:HD2	3:A:601:VVE:C2	2.04	0.86
1:C:225:PRO:HB2	1:C:226:PRO:HD3	1.58	0.85
1:C:451:LYS:HA	1:C:471:ASN:H	1.49	0.78
1:A:103:LYS:O	3:A:601:VVE:C2	2.36	0.73
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.70	0.73
1:C:253:THR:HA	1:C:292:VAL:HA	1.71	0.72
1:C:191:SER:OG	1:C:198:HIS:ND1	2.23	0.70
2:D:50:ILE:HG21	2:D:145:GLN:HB3	1.74	0.69
1:A:102:LYS:CD	3:A:601:VVE:C2	2.67	0.69
1:C:89:GLU:OE1	1:C:90:VAL:N	2.25	0.69
2:D:60:VAL:HG12	2:D:75:VAL:HG22	1.75	0.68
1:C:171:PHE:HB2	1:C:208:HIS:HD1	1.58	0.68
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.29	0.68
1:C:195:ILE:HG13	1:C:199:ARG:HH11	1.60	0.67
1:C:236:PRO:HA	3:C:601:VVE:O1	1.94	0.67
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.30	0.66
1:A:223:LYS:O	1:A:226:PRO:HD2	1.95	0.66
1:A:102:LYS:HD2	3:A:601:VVE:O2	1.96	0.64
2:B:156:SER:N	2:B:157:PRO:HD2	2.13	0.63
1:C:59:PRO:HG2	1:C:76:ASP:H	1.63	0.62
1:C:233:GLU:HB3	1:C:235:HIS:CE1	2.34	0.62
1:C:225:PRO:HB2	1:C:226:PRO:CD	2.30	0.62
2:D:373:GLN:NE2	2:D:406:TRP:O	2.32	0.62
1:A:194:GLU:HG2	1:A:197:GLN:H	1.64	0.62
1:C:227:PHE:CB	1:C:234:LEU:H	2.13	0.62
1:A:363:ASN:OD1	1:A:363:ASN:C	2.42	0.61
1:C:218:ASP:OD1	1:C:220:LYS:HD2	2.00	0.61
1:C:181:TYR:CD1	2:D:138:GLU:HB3	2.35	0.61
1:C:223:LYS:C	1:C:226:PRO:HD2	2.25	0.61
1:A:102:LYS:HE2	1:A:236:PRO:O	2.01	0.60
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.82	0.60
1:A:134:SER:HB3	1:A:139:THR:O	2.00	0.60
2:B:422:LEU:O	2:B:423:VAL:C	2.44	0.60
1:C:218:ASP:O	1:C:220:LYS:HG3	2.01	0.60
1:A:402:TRP:CD1	1:A:402:TRP:C	2.80	0.60
2:D:88:TRP:CB	2:D:154:LYS:HE2	2.31	0.60
1:C:227:PHE:CB	1:C:234:LEU:N	2.65	0.60
1:C:89:GLU:OE1	1:C:91:GLN:N	2.35	0.59
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LYS:H	1:C:226:PRO:HG2	1.68	0.59
1:A:3:SER:OG	1:A:5:ILE:HG22	2.03	0.59
1:A:105:SER:HB2	1:A:198:HIS:CD2	2.38	0.59
2:D:211:ARG:O	2:D:211:ARG:HG3	2.03	0.58
2:D:325:LEU:HD23	2:D:343:GLN:HG3	1.84	0.58
2:B:425:LEU:O	2:B:427:TYR:N	2.37	0.58
2:D:85:GLN:O	2:D:89:GLU:N	2.26	0.58
1:A:134:SER:CB	1:A:139:THR:O	2.52	0.58
1:C:501:TYR:CZ	1:C:505:ILE:HD11	2.38	0.58
1:A:473:THR:HG22	1:A:476:LYS:HE3	1.86	0.58
1:A:320:ASP:OD1	1:A:322:SER:OG	2.20	0.57
2:B:194:GLU:HB3	2:B:197:GLN:HG3	1.85	0.57
1:C:32:LYS:HA	1:C:35:VAL:HG12	1.86	0.57
1:C:524:GLN:O	1:C:528:LYS:HG2	2.04	0.57
2:D:25:PRO:C	2:D:26:LEU:HD12	2.29	0.57
1:A:7:THR:HG23	1:A:119:PRO:HB2	1.87	0.57
1:C:484:LEU:HA	1:C:487:GLN:HE21	1.70	0.57
1:C:97:PRO:HG2	1:C:232:TYR:CD1	2.39	0.56
1:C:93:GLY:C	1:C:94:ILE:HD13	2.30	0.56
2:D:387:PRO:HG2	2:D:389:PHE:CE1	2.40	0.56
1:A:332:GLN:O	1:A:336:GLN:HB2	2.05	0.56
2:D:425:LEU:O	2:D:426:TRP:C	2.48	0.56
1:C:150:PRO:HB2	1:C:153:TRP:HB2	1.87	0.56
1:C:203:GLU:OE2	1:C:206:ARG:NH1	2.38	0.56
2:D:156:SER:HB2	2:D:157:PRO:HD3	1.88	0.56
1:C:171:PHE:HB2	1:C:208:HIS:ND1	2.20	0.56
1:A:425:LEU:HD13	1:A:428:GLN:HE21	1.70	0.56
1:A:224:GLU:O	1:A:225:PRO:C	2.50	0.56
1:C:327:ALA:HB3	1:C:389:PHE:CD1	2.41	0.56
2:B:183:TYR:CE2	2:B:184:MET:HE3	2.41	0.55
1:A:156:SER:N	1:A:157:PRO:CD	2.69	0.55
3:C:601:VVE:C1	3:C:601:VVE:C4	2.84	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.89	0.55
2:B:313:PRO:HB2	2:B:315:HIS:CE1	2.42	0.55
1:A:306:ASN:HA	1:A:309:ILE:HD12	1.88	0.55
1:C:510:PRO:HB2	1:C:522:ILE:HD11	1.88	0.55
1:C:451:LYS:O	1:C:470:THR:HA	2.07	0.54
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.42	0.54
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.43	0.54
1:A:459:THR:HG22	1:A:463:ARG:N	2.23	0.54
2:B:85:GLN:O	2:B:89:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:O	2:B:184:MET:C	2.51	0.53
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.43	0.53
1:C:233:GLU:HB3	1:C:235:HIS:NE2	2.24	0.53
1:C:181:TYR:CE1	2:D:138:GLU:HB3	2.43	0.53
1:C:169:GLU:HB2	1:C:170:PRO:HD3	1.91	0.53
2:D:136:ASN:O	2:D:137:ASN:C	2.52	0.53
2:D:296:THR:HG22	2:D:299:ALA:H	1.74	0.53
2:B:184:MET:O	2:B:185:ASP:HB2	2.09	0.53
2:B:425:LEU:O	2:B:426:TRP:C	2.52	0.53
1:C:447:ASN:OD1	1:C:449:GLU:HB3	2.08	0.52
1:A:425:LEU:HD13	1:A:428:GLN:NE2	2.23	0.52
1:C:544:GLY:O	1:C:545:ASN:C	2.52	0.52
2:B:342:TYR:CD1	2:B:342:TYR:C	2.87	0.52
1:C:505:ILE:O	1:C:508:ALA:HB3	2.09	0.52
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.92	0.52
2:B:232:TYR:CG	2:B:233:GLU:N	2.76	0.52
1:A:303:LEU:O	1:A:307:ARG:HG3	2.10	0.52
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.45	0.52
2:B:325:LEU:C	2:B:326:ILE:HD12	2.35	0.51
2:B:203:GLU:O	2:B:207:GLN:HG2	2.10	0.51
1:A:218:ASP:HA	1:A:221:HIS:NE2	2.25	0.51
1:A:486:LEU:O	1:A:489:SER:HB2	2.10	0.51
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.92	0.51
2:D:368:LEU:O	2:D:372:VAL:HG23	2.10	0.51
2:D:182:GLN:CA	2:D:187:LEU:HA	2.25	0.51
2:D:336:GLN:C	2:D:337:TRP:CD1	2.89	0.51
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.46	0.51
2:D:75:VAL:HG11	2:D:77:PHE:CZ	2.46	0.51
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.92	0.50
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.94	0.50
1:C:438:GLU:OE2	1:C:463:ARG:HD3	2.12	0.50
1:A:181:TYR:CE1	2:B:138:GLU:HB3	2.47	0.50
2:B:388:LYS:HG3	2:B:413:GLU:HB3	1.93	0.50
1:C:3:SER:N	1:C:4:PRO:CD	2.74	0.50
2:B:249:LYS:HD2	2:B:252:TRP:CE3	2.47	0.50
1:C:240:THR:OG1	1:C:241:VAL:N	2.43	0.50
2:D:75:VAL:HG11	2:D:77:PHE:CE2	2.47	0.50
2:D:239:TRP:CZ2	2:D:378:GLU:HG2	2.47	0.50
1:C:8:VAL:O	1:C:121:ASP:HB2	2.12	0.49
1:A:70:LYS:O	1:A:71:TRP:HB2	2.11	0.49
1:A:135:ILE:H	1:A:135:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:O	2:B:307:ARG:HG3	2.12	0.49
1:C:35:VAL:HA	1:C:38:CYS:HB2	1.94	0.49
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.93	0.49
1:A:393:ILE:HG23	1:A:393:ILE:O	2.11	0.49
2:D:119:PRO:HA	2:D:148:VAL:HA	1.95	0.49
2:B:344:GLU:HB3	2:B:345:PRO:HD2	1.94	0.49
2:D:153:TRP:CZ3	2:D:155:GLY:HA3	2.48	0.49
1:C:473:THR:O	1:C:474:ASN:C	2.55	0.48
1:C:549:ASP:O	1:C:553:SER:N	2.45	0.48
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.43	0.48
2:B:163:SER:O	2:B:167:ILE:HG13	2.12	0.48
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.49	0.48
2:B:382:ILE:HG22	2:B:383:TRP:CD2	2.48	0.48
2:D:281:LYS:O	2:D:284:ARG:HD2	2.12	0.48
1:C:254:VAL:HG23	1:C:291:GLU:HG3	1.95	0.48
1:A:123:ASP:N	1:A:123:ASP:OD1	2.45	0.48
2:B:198:HIS:C	2:B:198:HIS:CD2	2.91	0.48
1:A:427:TYR:O	1:A:428:GLN:HG2	2.14	0.48
1:C:180:ILE:HG12	1:C:189:VAL:HG22	1.96	0.48
1:A:491:LEU:HD23	1:A:529:GLU:CD	2.39	0.48
2:D:365:VAL:HG12	2:D:405:TYR:HE1	1.77	0.48
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.95	0.48
2:B:382:ILE:HG22	2:B:383:TRP:CG	2.49	0.48
1:C:32:LYS:O	1:C:36:GLU:N	2.47	0.48
2:D:330:GLN:NE2	2:D:338:THR:OG1	2.42	0.48
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.49	0.47
1:C:183:TYR:HD2	1:C:188:TYR:OH	1.97	0.47
1:A:28:GLU:HA	1:A:31:ILE:HG13	1.95	0.47
1:C:24:TRP:N	1:C:25:PRO:HD3	2.29	0.47
1:A:94:ILE:HG22	1:A:183:TYR:CE1	2.50	0.47
2:B:105:SER:HB2	2:B:198:HIS:ND1	2.30	0.47
1:C:522:ILE:O	1:C:523:GLU:C	2.57	0.47
1:A:206:ARG:CZ	1:A:218:ASP:HB2	2.45	0.47
1:A:540:LYS:HA	1:A:540:LYS:HD2	1.59	0.47
2:B:54:ASN:O	2:B:143:ARG:NH2	2.48	0.47
1:C:9:PRO:HA	1:C:121:ASP:OD2	2.14	0.47
2:D:20:LYS:O	2:D:20:LYS:HD3	2.15	0.47
2:D:157:PRO:HG2	2:D:184:MET:HA	1.96	0.47
2:D:169:GLU:N	2:D:170:PRO:CD	2.78	0.47
1:C:94:ILE:HG22	1:C:95:PRO:O	2.14	0.47
2:B:326:ILE:HG21	2:B:342:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:O	1:C:184:MET:C	2.56	0.47
2:B:425:LEU:C	2:B:427:TYR:N	2.73	0.47
2:D:334:GLN:OE1	2:D:334:GLN:HA	2.14	0.46
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.16	0.46
1:C:101:LYS:O	1:C:103:LYS:HG2	2.16	0.46
2:B:85:GLN:HG3	2:B:86:ASP:N	2.28	0.46
2:D:380:ILE:O	2:D:384:GLY:N	2.46	0.46
1:A:379:SER:CB	1:A:387:PRO:HD3	2.46	0.46
1:C:465:LYS:O	1:C:466:VAL:HB	2.15	0.46
1:C:97:PRO:HG2	1:C:232:TYR:CG	2.51	0.46
2:B:104:LYS:O	2:B:235:HIS:HA	2.15	0.46
2:B:172:LYS:HB2	2:B:172:LYS:HE3	1.60	0.46
1:C:84:THR:HB	1:C:154:LYS:HD3	1.97	0.46
1:A:179:VAL:HB	3:A:601:VVE:CL1	2.53	0.46
2:B:183:TYR:OH	2:B:386:THR:HG23	2.17	0.45
1:C:171:PHE:CZ	1:C:205:LEU:HB2	2.51	0.45
1:C:254:VAL:HG23	1:C:291:GLU:O	2.17	0.45
1:C:64:LYS:HA	1:C:70:LYS:O	2.17	0.45
1:C:96:HIS:H	2:D:136:ASN:ND2	2.14	0.45
2:D:50:ILE:CG2	2:D:145:GLN:HB3	2.45	0.45
1:A:65:LYS:HA	1:A:65:LYS:HD2	1.58	0.45
2:D:27:THR:CG2	2:D:30:LYS:HD3	2.47	0.45
1:A:473:THR:CG2	1:A:476:LYS:HE3	2.47	0.45
1:C:225:PRO:CB	1:C:226:PRO:CD	2.94	0.45
1:C:379:SER:HB3	1:C:385:LYS:O	2.16	0.45
1:A:29:GLU:HG3	1:A:30:LYS:N	2.31	0.45
1:A:245:VAL:O	1:A:246:LEU:CB	2.65	0.45
2:D:252:TRP:HA	2:D:252:TRP:CE3	2.51	0.45
1:A:120:LEU:O	1:A:121:ASP:C	2.59	0.45
1:C:94:ILE:HG23	1:C:229:TRP:CH2	2.52	0.45
1:C:96:HIS:H	2:D:136:ASN:CG	2.25	0.45
2:D:296:THR:HB	2:D:299:ALA:HB2	1.99	0.45
1:A:53:GLU:HG2	1:A:54:ASN:N	2.31	0.44
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.46	0.44
1:C:121:ASP:OD1	1:C:122:GLU:N	2.50	0.44
1:C:501:TYR:CE1	1:C:505:ILE:HD11	2.52	0.44
2:D:125:ARG:O	2:D:126:LYS:C	2.61	0.44
1:A:553:SER:O	1:A:554:ALA:C	2.60	0.44
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.98	0.44
2:B:371:ALA:O	2:B:374:LYS:N	2.50	0.44
1:C:450:THR:C	1:C:452:LEU:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LEU:O	2:D:121:ASP:C	2.61	0.44
2:D:183:TYR:N	2:D:186:ASP:O	2.45	0.44
2:D:24:TRP:N	2:D:24:TRP:CD1	2.84	0.44
1:A:37:ILE:O	1:A:41:MET:HG3	2.17	0.44
1:C:156:SER:N	1:C:157:PRO:CD	2.81	0.44
1:C:453:GLY:HA3	1:C:469:LEU:HB2	1.99	0.44
2:D:77:PHE:O	2:D:78:ARG:C	2.61	0.44
2:D:125:ARG:HD3	2:D:147:ASN:HA	2.00	0.44
2:D:24:TRP:O	2:D:26:LEU:CD1	2.66	0.44
1:A:354:TYR:HB2	1:A:374:LYS:HE2	2.00	0.43
1:A:3:SER:C	1:A:5:ILE:H	2.26	0.43
2:B:154:LYS:HE3	2:B:184:MET:HE2	1.99	0.43
2:B:216:THR:O	2:B:217:PRO:C	2.61	0.43
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.00	0.43
1:C:178:ILE:CG2	1:C:189:VAL:HG13	2.49	0.43
1:A:226:PRO:O	1:A:228:LEU:N	2.51	0.43
1:A:399:GLU:HA	1:A:402:TRP:CZ3	2.52	0.43
1:A:545:ASN:O	1:A:548:VAL:HG12	2.19	0.43
2:B:156:SER:N	2:B:157:PRO:CD	2.81	0.43
1:C:103:LYS:O	1:C:104:LYS:C	2.61	0.43
2:D:301:LEU:O	2:D:302:GLU:C	2.60	0.43
1:A:63:ILE:O	1:A:71:TRP:HA	2.19	0.43
1:A:476:LYS:HE3	1:A:476:LYS:HB2	1.80	0.43
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.49	0.43
1:A:545:ASN:HA	1:A:548:VAL:HG12	1.99	0.43
2:B:239:TRP:CZ3	2:B:378:GLU:HG2	2.53	0.43
1:C:32:LYS:O	1:C:35:VAL:HG12	2.18	0.43
1:A:479:LEU:HD11	1:A:521:ILE:CD1	2.48	0.43
1:C:94:ILE:CG2	1:C:229:TRP:CH2	3.02	0.43
1:C:303:LEU:O	1:C:307:ARG:HB2	2.18	0.43
2:B:263:LYS:HG3	2:B:426:TRP:HB2	1.99	0.43
1:C:366:LYS:O	1:C:369:THR:HB	2.19	0.43
1:C:473:THR:C	1:C:475:GLN:N	2.76	0.43
2:D:183:TYR:O	2:D:184:MET:C	2.62	0.43
1:A:135:ILE:H	1:A:135:ILE:CD1	2.32	0.43
1:A:455:ALA:HB2	1:A:469:LEU:HD11	2.00	0.43
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.54	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.53	0.43
1:C:509:GLN:N	1:C:510:PRO:HD3	2.34	0.43
2:D:68:SER:C	2:D:70:LYS:H	2.25	0.43
2:D:330:GLN:NE2	2:D:330:GLN:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ALA:HB3	1:C:291:GLU:HB3	2.01	0.42
1:C:149:LEU:HD11	1:C:159:ILE:HG22	2.00	0.42
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.54	0.42
1:C:95:PRO:HG3	2:D:137:ASN:O	2.19	0.42
2:D:259:LYS:O	2:D:260:LEU:C	2.63	0.42
1:A:374:LYS:HG3	1:A:375:ILE:N	2.35	0.42
2:B:64:LYS:HG3	2:B:70:LYS:O	2.19	0.42
2:B:424:LYS:O	2:B:425:LEU:C	2.62	0.42
2:D:345:PRO:C	2:D:347:LYS:H	2.26	0.42
1:A:236:PRO:HA	3:A:601:VVE:C24	2.49	0.42
1:C:225:PRO:CB	1:C:226:PRO:HD3	2.39	0.42
1:A:112:GLY:O	1:A:113:ASP:C	2.62	0.42
1:A:382:ILE:O	2:B:136:ASN:HB2	2.20	0.42
1:A:26:LEU:O	1:A:27:THR:C	2.63	0.42
1:C:59:PRO:HG3	1:C:76:ASP:HB3	2.02	0.42
1:C:218:ASP:CG	1:C:220:LYS:HD2	2.44	0.42
1:C:235:HIS:HA	1:C:236:PRO:HD3	1.92	0.42
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.19	0.42
1:A:102:LYS:HA	3:A:601:VVE:O2	2.20	0.42
1:C:179:VAL:HG11	3:C:601:VVE:CL1	2.56	0.42
1:C:544:GLY:HA2	1:C:547:GLN:OE1	2.19	0.42
1:A:60:VAL:HG22	1:A:61:PHE:N	2.34	0.41
1:A:398:TRP:CD1	1:A:402:TRP:CE3	3.07	0.41
1:C:102:LYS:HA	3:C:601:VVE:O2	2.19	0.41
1:C:478:GLU:O	1:C:482:ILE:HG12	2.20	0.41
1:A:100:LEU:HB3	3:A:601:VVE:C6	2.50	0.41
1:C:235:HIS:HB2	1:C:238:LYS:O	2.20	0.41
1:C:325:LEU:HD12	1:C:325:LEU:HA	1.74	0.41
2:D:168:LEU:HA	2:D:208:HIS:HE1	1.84	0.41
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.55	0.41
1:C:100:LEU:HD13	3:C:601:VVE:C19	2.49	0.41
1:C:236:PRO:O	1:C:237:ASP:CB	2.68	0.41
1:A:233:GLU:HB3	1:A:235:HIS:NE2	2.35	0.41
1:A:255:ASN:HA	1:A:258:GLN:HG3	2.03	0.41
1:C:486:LEU:O	1:C:528:LYS:NZ	2.54	0.41
2:D:125:ARG:HD3	2:D:146:TYR:O	2.21	0.41
1:A:245:VAL:O	1:A:246:LEU:HB3	2.21	0.41
1:C:296:THR:O	1:C:299:ALA:HB3	2.20	0.41
1:A:29:GLU:HG3	1:A:30:LYS:H	1.85	0.41
1:A:458:VAL:HG12	2:B:286:THR:HG21	2.02	0.41
2:B:167:ILE:O	2:B:208:HIS:NE2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:GLY:O	2:D:156:SER:C	2.63	0.41
1:A:149:LEU:HB3	1:A:156:SER:OG	2.20	0.41
1:A:515:SER:O	1:A:516:GLU:C	2.63	0.41
1:C:108:VAL:HG23	1:C:188:TYR:HD1	1.85	0.41
1:C:205:LEU:O	1:C:206:ARG:C	2.62	0.41
2:D:337:TRP:CZ3	2:D:368:LEU:HD13	2.56	0.41
1:A:139:THR:O	1:A:140:PRO:C	2.63	0.41
2:B:339:TYR:C	2:B:340:GLN:NE2	2.78	0.41
2:B:371:ALA:O	2:B:372:VAL:C	2.63	0.41
1:C:108:VAL:HG23	1:C:188:TYR:CD1	2.55	0.41
1:C:184:MET:O	1:C:185:ASP:C	2.63	0.41
1:C:538:ALA:O	1:C:539:HIS:C	2.63	0.41
1:C:552:VAL:O	1:C:553:SER:C	2.62	0.41
2:D:117:SER:O	2:D:118:VAL:C	2.63	0.41
2:D:296:THR:HG22	2:D:298:GLU:N	2.36	0.41
1:A:113:ASP:O	1:A:114:ALA:C	2.64	0.41
1:A:254:VAL:HG23	1:A:291:GLU:O	2.21	0.41
1:A:459:THR:HG22	1:A:463:ARG:H	1.87	0.41
1:A:465:LYS:HG2	1:A:466:VAL:N	2.36	0.41
2:B:58:THR:HG21	2:B:77:PHE:CD1	2.55	0.41
2:B:239:TRP:CH2	2:B:378:GLU:HG3	2.56	0.41
2:B:340:GLN:N	2:B:340:GLN:CD	2.78	0.41
1:C:326:ILE:O	1:C:341:ILE:HA	2.21	0.41
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.56	0.40
1:C:3:SER:N	1:C:4:PRO:HD2	2.35	0.40
1:A:79:GLU:O	1:A:80:LEU:C	2.64	0.40
1:A:496:VAL:HG21	2:B:289:LEU:HD21	2.02	0.40
1:C:175:ASN:HB3	1:C:178:ILE:HG12	2.03	0.40
1:C:268:SER:O	1:C:351:THR:O	2.39	0.40
1:C:473:THR:O	1:C:476:LYS:N	2.54	0.40
2:D:420:PRO:HB2	2:D:421:PRO:CD	2.52	0.40
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.04	0.40
2:B:319:TYR:OH	2:B:385:LYS:HD2	2.20	0.40
2:B:388:LYS:CG	2:B:413:GLU:HB3	2.50	0.40
1:C:291:GLU:HG3	1:C:291:GLU:O	2.20	0.40
1:C:545:ASN:O	1:C:549:ASP:HB2	2.22	0.40
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.57	0.40
2:B:110:ASP:HB3	2:B:217:PRO:HG2	2.03	0.40
2:D:124:PHE:O	2:D:125:ARG:C	2.64	0.40
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.39	0.40
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HD23	1:C:187:LEU:HA	1.81	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	546/556 (98%)	512 (94%)	32 (6%)	2 (0%)	30	65
1	C	516/556 (93%)	465 (90%)	50 (10%)	1 (0%)	43	76
2	B	395/428 (92%)	374 (95%)	19 (5%)	2 (0%)	24	60
2	D	388/428 (91%)	339 (87%)	49 (13%)	0	100	100
All	All	1845/1968 (94%)	1690 (92%)	150 (8%)	5 (0%)	36	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	426	TRP
1	C	237	ASP
2	B	184	MET
1	A	226	PRO
1	A	225	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	417/495 (84%)	364 (87%)	53 (13%)	4	20
1	C	328/495 (66%)	300 (92%)	28 (8%)	10	36
2	B	340/390 (87%)	306 (90%)	34 (10%)	7	29
2	D	224/390 (57%)	194 (87%)	30 (13%)	4	18
All	All	1309/1770 (74%)	1164 (89%)	145 (11%)	6	25

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	THR
1	A	11	LYS
1	A	16	MET
1	A	21	VAL
1	A	23	GLN
1	A	31	ILE
1	A	42	GLU
1	A	46	LYS
1	A	58	THR
1	A	63	ILE
1	A	65	LYS
1	A	68	SER
1	A	103	LYS
1	A	105	SER
1	A	123	ASP
1	A	126	LYS
1	A	135	ILE
1	A	139	THR
1	A	151	GLN
1	A	162	SER
1	A	163	SER
1	A	178	ILE
1	A	194	GLU
1	A	216	THR
1	A	219	LYS
1	A	225	PRO
1	A	241	VAL
1	A	244	ILE
1	A	245	VAL
1	A	258	GLN
1	A	292	VAL
1	A	296	THR

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Mol	Chain	Res	Type
1	A	332	GLN
1	A	362	THR
1	A	363	ASN
1	A	374	LYS
1	A	386	THR
1	A	393	ILE
1	A	400	THR
1	A	402	TRP
1	A	413	GLU
1	A	415	GLU
1	A	459	THR
1	A	467	VAL
1	A	482	ILE
1	A	489	SER
1	A	491	LEU
1	A	513	SER
1	A	527	LYS
1	A	540	LYS
1	A	542	ILE
1	A	547	GLN
2	B	21	VAL
2	B	24	TRP
2	B	55	PRO
2	B	58	THR
2	B	64	LYS
2	B	84	THR
2	B	85	GLN
2	B	86	ASP
2	B	89	GLU
2	B	92	LEU
2	B	134	SER
2	B	163	SER
2	B	167	ILE
2	B	172	LYS
2	B	175	ASN
2	B	184	MET
2	B	185	ASP
2	B	193	LEU
2	B	195	ILE
2	B	200	THR
2	B	216	THR
2	B	218	ASP

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Mol	Chain	Res	Type
2	B	233	GLU
2	B	242	GLN
2	B	249	LYS
2	B	253	THR
2	B	254	VAL
2	B	290	THR
2	B	314	VAL
2	B	321	PRO
2	B	338	THR
2	B	417	VAL
2	B	418	ASN
2	B	427	TYR
1	C	35	VAL
1	C	38	CYS
1	C	94	ILE
1	C	101	LYS
1	C	106	VAL
1	C	107	THR
1	C	111	VAL
1	C	113	ASP
1	C	123	ASP
1	C	161	GLN
1	C	184	MET
1	C	186	ASP
1	C	200	THR
1	C	203	GLU
1	C	219	LYS
1	C	220	LYS
1	C	291	GLU
1	C	325	LEU
1	C	351	THR
1	C	393	ILE
1	C	442	VAL
1	C	447	ASN
1	C	449	GLU
1	C	454	LYS
1	C	473	THR
1	C	493	VAL
1	C	496	VAL
1	C	527	LYS
2	D	20	LYS
2	D	27	THR

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Mol	Chain	Res	Type
2	D	48	SER
2	D	63	ILE
2	D	68	SER
2	D	101	LYS
2	D	125	ARG
2	D	126	LYS
2	D	135	ILE
2	D	137	ASN
2	D	139	THR
2	D	147	ASN
2	D	175	ASN
2	D	237	ASP
2	D	252	TRP
2	D	253	THR
2	D	274	ILE
2	D	284	ARG
2	D	293	ILE
2	D	296	THR
2	D	314	VAL
2	D	317	VAL
2	D	330	GLN
2	D	361	HIS
2	D	405	TYR
2	D	410	TRP
2	D	417	VAL
2	D	423	VAL
2	D	425	LEU
2	D	426	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	235	HIS
1	A	269	GLN
1	A	315	HIS
1	A	394	GLN
2	B	197	GLN
2	B	235	HIS
2	B	242	GLN
2	B	269	GLN
2	B	315	HIS

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Mol	Chain	Res	Type
2	B	330	GLN
2	B	334	GLN
2	B	340	GLN
1	C	161	GLN
1	C	175	ASN
1	C	182	GLN
1	C	269	GLN
1	C	487	GLN
2	D	208	HIS
2	D	330	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	A	602	-	4,4,4	0.76	0	6,6,6	0.47	0
3	VVE	C	601	-	37,37,37	0.98	2 (5%)	49,52,52	1.16	1 (2%)
3	VVE	A	601	-	37,37,37	0.51	0	49,52,52	1.65	5 (10%)
4	PO4	B	501	-	4,4,4	0.74	0	6,6,6	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VVE	C	601	-	-	6/18/18/18	0/4/4/4
3	VVE	A	601	-	-	4/18/18/18	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	VVE	C1-C2	-4.99	1.30	1.51
3	C	601	VVE	C2-C3	-2.18	1.47	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VVE	C1-C2-C3	8.21	127.07	112.69
3	C	601	VVE	C1-C2-C3	6.73	124.48	112.69
3	A	601	VVE	O3-C7-C12	4.14	124.30	115.75
3	A	601	VVE	O3-C7-C8	-4.08	114.68	123.49
3	A	601	VVE	C6-O3-C7	2.34	123.34	117.69
3	A	601	VVE	C5-N2-C4	2.23	125.93	121.81

There are no chirality outliers.

All (10) torsion outliers are listed below:

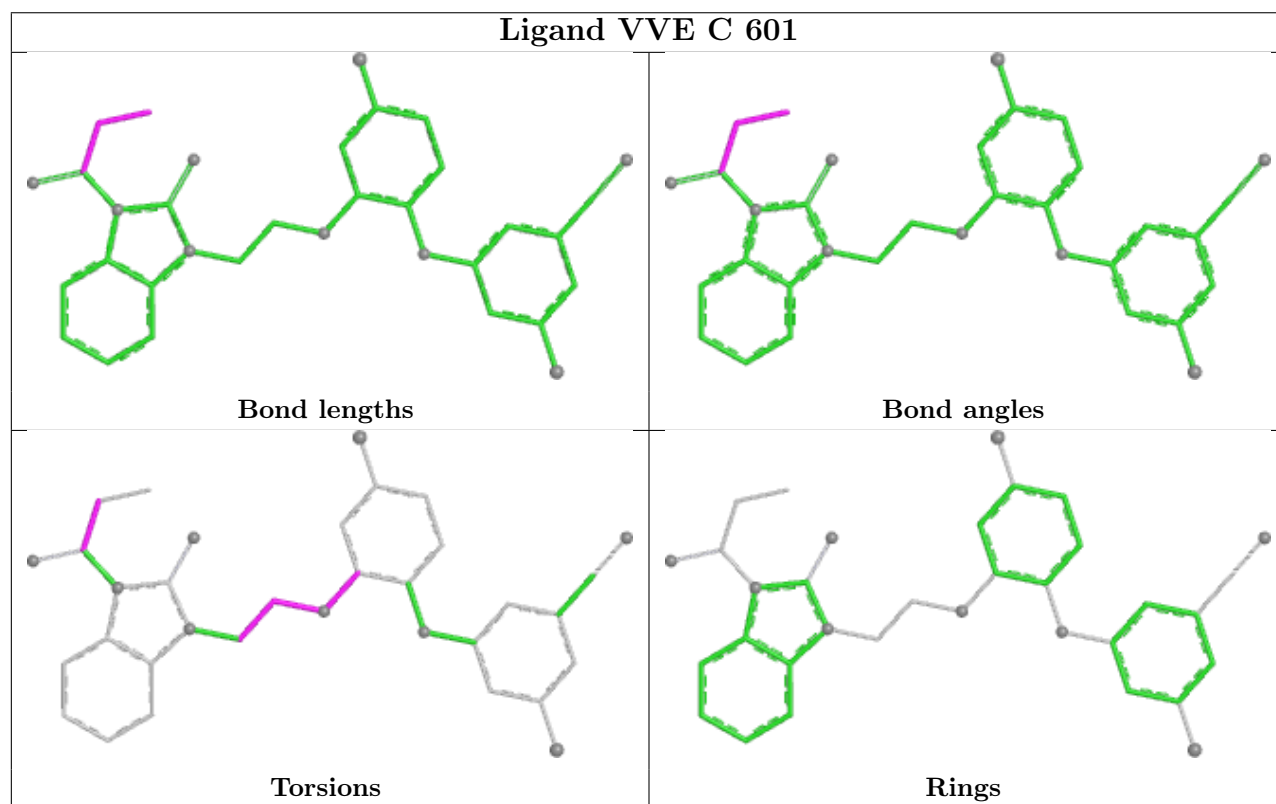
Mol	Chain	Res	Type	Atoms
3	C	601	VVE	C1-C2-C3-O1
3	C	601	VVE	C1-C2-C3-N1
3	A	601	VVE	C8-C7-O3-C6
3	A	601	VVE	C12-C7-O3-C6
3	C	601	VVE	N2-C5-C6-O3
3	A	601	VVE	C6-C5-N2-C4
3	C	601	VVE	C5-C6-O3-C7
3	C	601	VVE	C12-C7-O3-C6
3	A	601	VVE	C6-C5-N2-C20
3	C	601	VVE	C8-C7-O3-C6

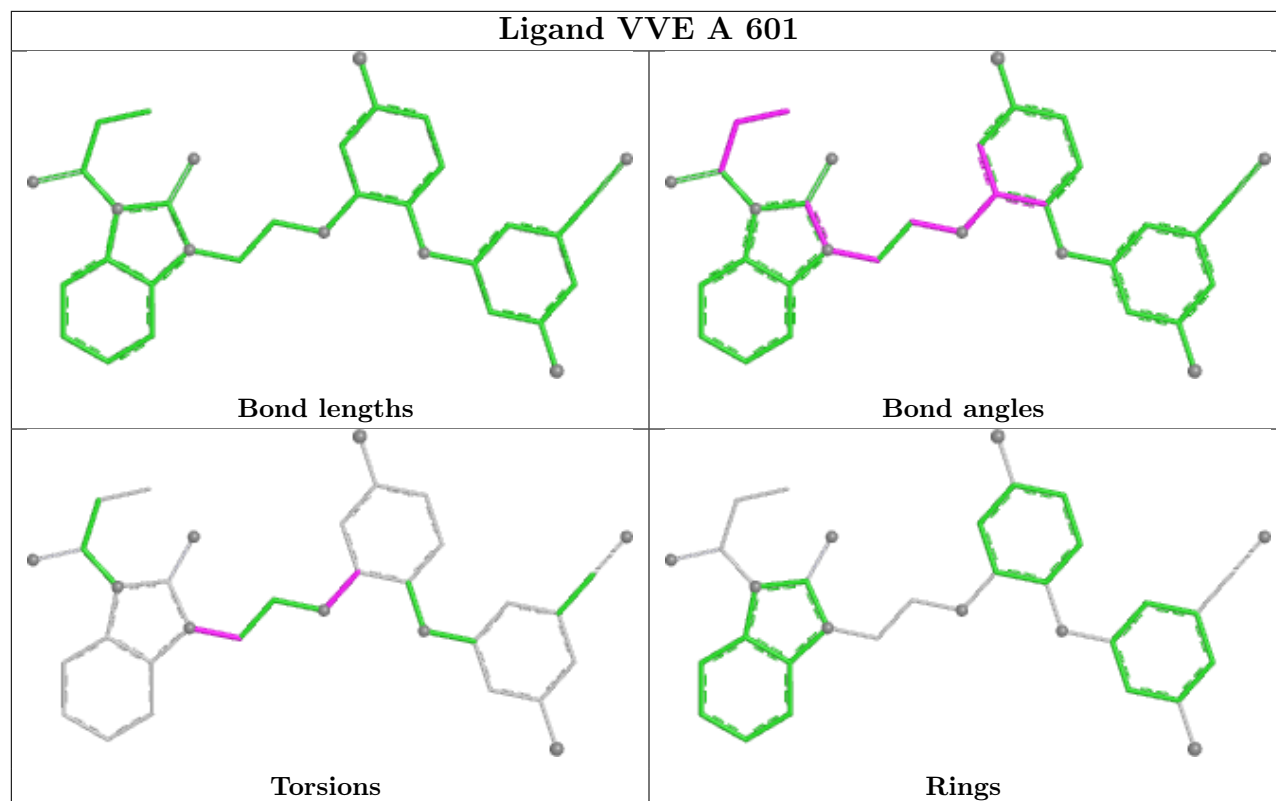
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	VVE	6	0
3	A	601	VVE	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	550/556 (98%)	0.22	20 (3%)	46	26	30, 76, 143, 200	0
1	C	531/556 (95%)	0.78	53 (9%)	12	7	30, 125, 186, 235	1 (0%)
2	B	403/428 (94%)	0.03	10 (2%)	58	35	38, 71, 120, 168	1 (0%)
2	D	395/428 (92%)	0.72	36 (9%)	15	8	30, 133, 183, 210	2 (0%)
All	All	1879/1968 (95%)	0.44	119 (6%)	26	13	30, 102, 173, 235	4 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	7	THR	6.9
2	D	6	GLU	6.6
1	C	25	PRO	6.0
1	C	224	GLU	5.5
1	C	146	TYR	5.5
2	D	114	ALA	5.5
1	C	225	PRO	5.4
1	C	130	PHE	5.2
1	C	24	TRP	5.0
1	C	128	THR	4.9
1	A	3	SER	4.8
1	C	533	LEU	4.6
1	C	285	GLY	4.5
1	C	150	PRO	4.4
1	C	234	LEU	4.1
2	B	363	ASN	4.0
1	A	276	VAL	4.0
2	D	5	ILE	3.9
1	C	144	TYR	3.7
1	C	23	GLN	3.7
1	C	337	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	426	TRP	3.7
2	D	280	SER	3.6
1	C	252	TRP	3.6
1	C	67	ASP	3.5
2	B	284	ARG	3.5
2	D	184	MET	3.5
1	C	19	PRO	3.5
1	C	226	PRO	3.5
2	D	375	ILE	3.4
1	C	412	PRO	3.3
2	B	88	TRP	3.3
2	D	383	TRP	3.3
2	B	427	TYR	3.3
1	C	236	PRO	3.3
2	D	127	TYR	3.2
1	C	152	GLY	3.2
1	A	69	THR	3.1
1	C	188	TYR	3.1
1	C	272	PRO	3.1
1	A	246	LEU	3.0
1	C	129	ALA	3.0
2	D	124	PHE	3.0
1	A	65	LYS	3.0
2	D	185	ASP	3.0
1	C	100	LEU	2.9
1	C	38	CYS	2.9
2	D	425	LEU	2.9
2	D	142	ILE	2.9
2	D	284	ARG	2.8
1	A	344	GLU	2.8
1	C	223	LYS	2.8
1	C	294	PRO	2.8
1	C	534	ALA	2.8
1	C	149	LEU	2.8
2	D	303	LEU	2.8
2	B	428	GLN	2.8
1	C	181	TYR	2.8
1	C	108	VAL	2.7
2	D	8	VAL	2.7
1	A	64	LYS	2.7
1	A	299	ALA	2.6
1	C	554	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	247	PRO	2.6
2	D	299	ALA	2.6
2	D	379	SER	2.6
1	A	413	GLU	2.5
1	C	132	ILE	2.5
1	C	127	TYR	2.5
1	C	318	TYR	2.5
1	A	2	ILE	2.5
2	D	283	LEU	2.4
1	C	270	ILE	2.4
2	D	421	PRO	2.4
1	A	70	LYS	2.3
2	D	38	CYS	2.3
1	A	332	GLN	2.3
1	C	427	TYR	2.3
1	A	225	PRO	2.3
2	B	232	TYR	2.3
1	C	114	ALA	2.3
1	C	279	LEU	2.3
1	A	5	ILE	2.3
2	D	354	TYR	2.3
1	A	552	VAL	2.3
1	A	551	LEU	2.3
2	D	242	GLN	2.3
1	C	229	TRP	2.2
1	C	119	PRO	2.2
1	C	314	VAL	2.2
2	D	405	TYR	2.2
1	C	77	PHE	2.2
1	A	66	LYS	2.2
1	C	102	LYS	2.2
1	A	135	ILE	2.2
2	D	271	TYR	2.2
2	D	37	ILE	2.2
2	D	426	TRP	2.2
2	D	160	PHE	2.2
1	C	282	LEU	2.2
2	D	276	VAL	2.2
1	C	103	LYS	2.2
2	D	260	LEU	2.2
1	C	235	HIS	2.1
1	A	286	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	408	ALA	2.1
2	D	278	GLN	2.1
1	C	34	LEU	2.1
2	B	195	ILE	2.1
2	D	99	GLY	2.1
1	C	101	LYS	2.1
2	B	273	GLY	2.1
1	C	237	ASP	2.1
2	D	410	TRP	2.1
1	A	298	GLU	2.1
2	D	186	ASP	2.0
2	D	266	TRP	2.0
2	B	87	PHE	2.0
1	C	339	TYR	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](#)

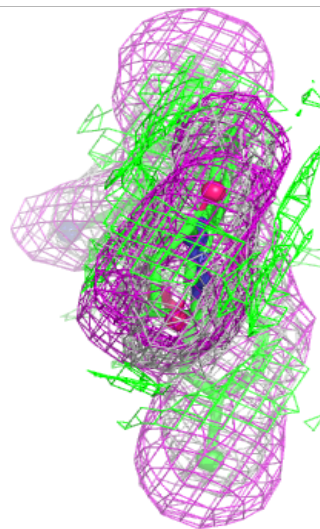
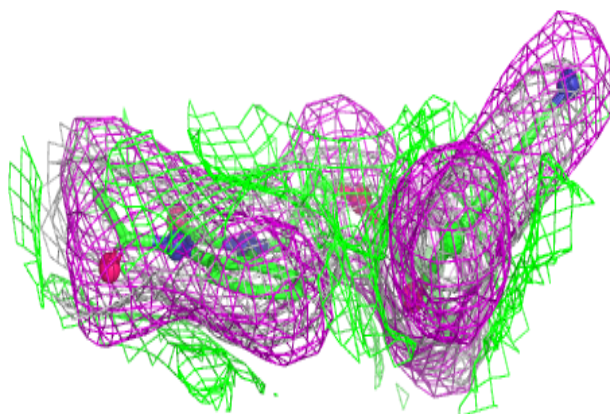
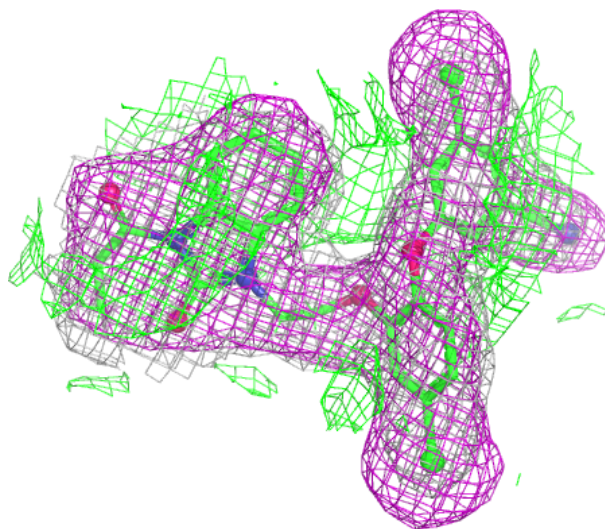
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VVE	C	601	34/34	0.75	0.15	0,0,0,0	0
3	VVE	A	601	34/34	0.92	0.12	48,62,101,110	0
4	PO4	B	501	5/5	0.92	0.39	30,30,30,30	0
4	PO4	A	602	5/5	0.93	0.38	30,30,30,30	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.

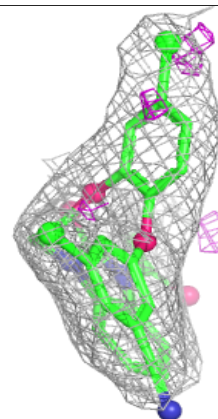
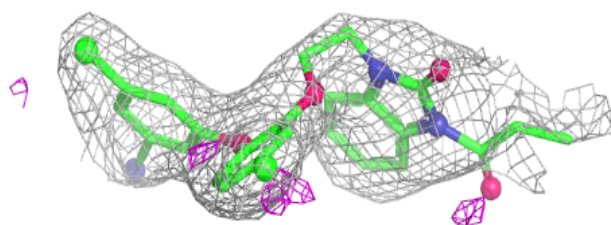
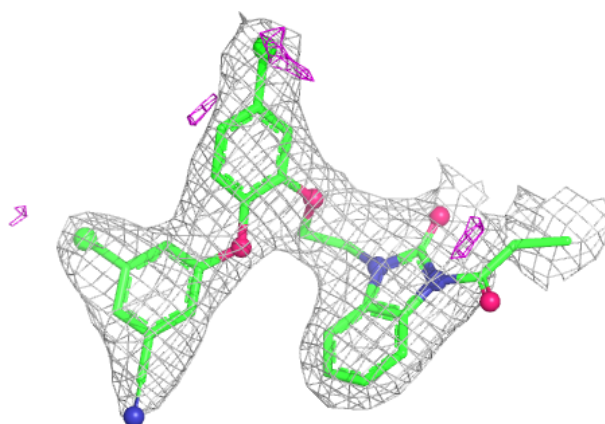
Electron density around VVE C 601:

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



Electron density around VVE A 601:

$2mF_o-DF_c$ (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.