



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:13 PM EDT

PDB ID : 1C1C  
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH TNK-6123  
Authors : Hopkins, A.L.; Ren, J.; Tanaka, H.; Baba, M.; Okamoto, M.; Stuart, D.I.; Stammers, D.K.  
Deposited on : 1999-07-21  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

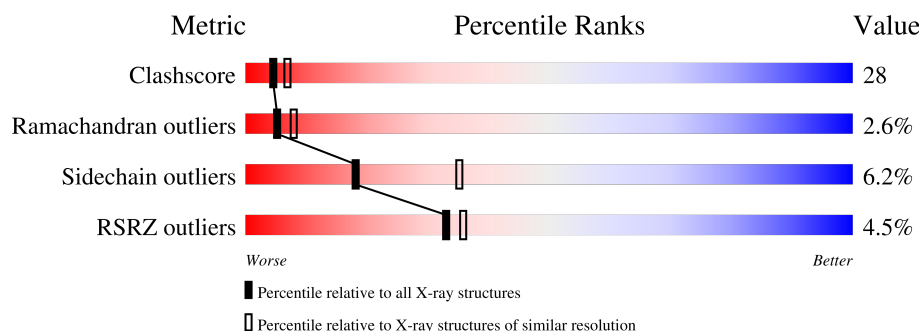
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div> <div>48%</div> <div>42%</div> <div>5%</div> </div> </div>
2	B	440	<div> <div>5%</div> <div> <div>46%</div> <div>45%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7997 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 HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4396	2846	732	810	8			

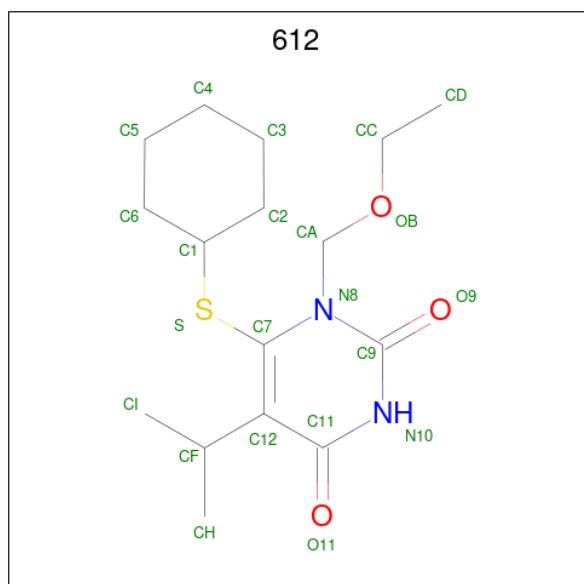
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	416	Total	C	N	O	S	0	0	0
			3437	2236	569	625	7			

- Molecule 3 is 6-(cyclohexylsulfanyl)-1-(ethoxymethyl)-5-(1-methylethyl)pyrimidine-2,4(1H, 3H)-dione (three-letter code: 612) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	16	2	3	1		

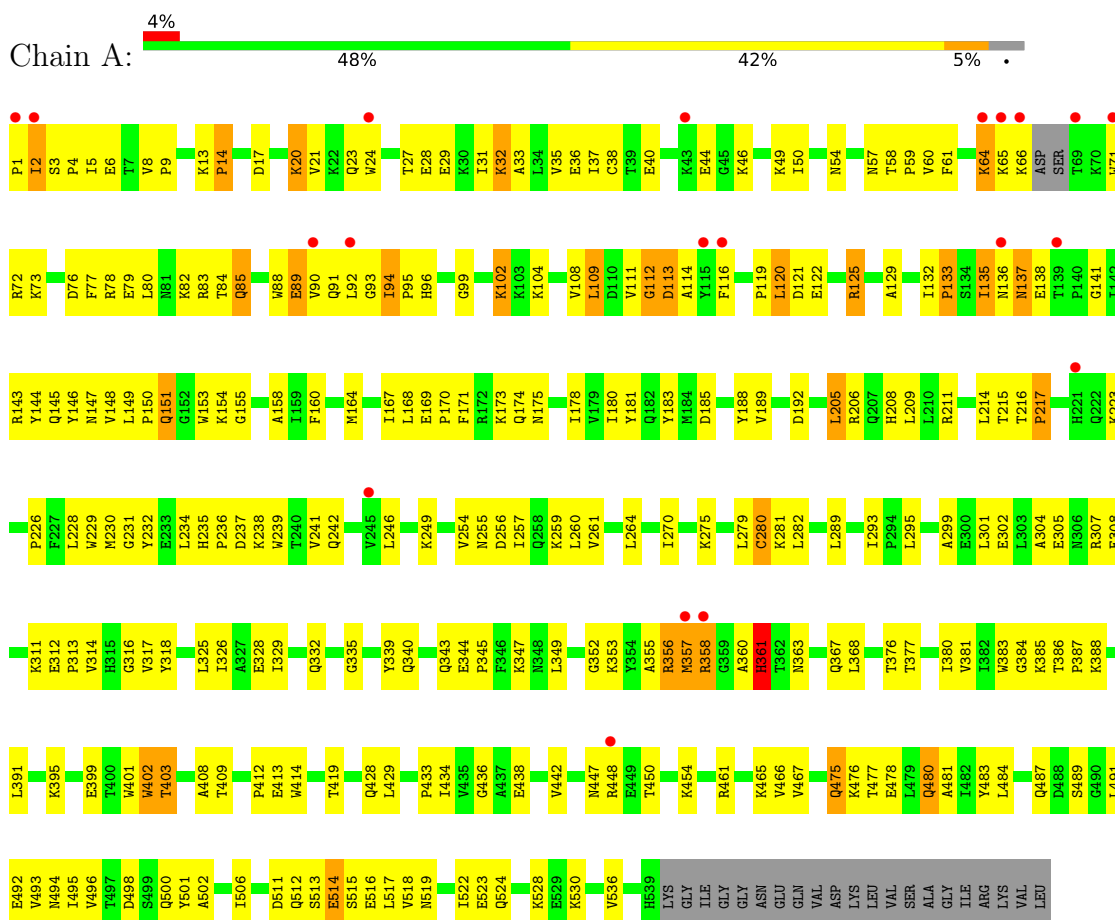
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	47	Total	O	0	0
			47	47		

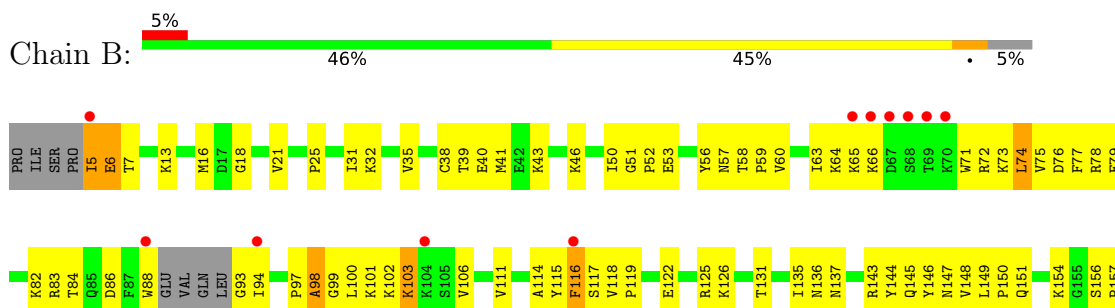
### 3 Residue-property plots

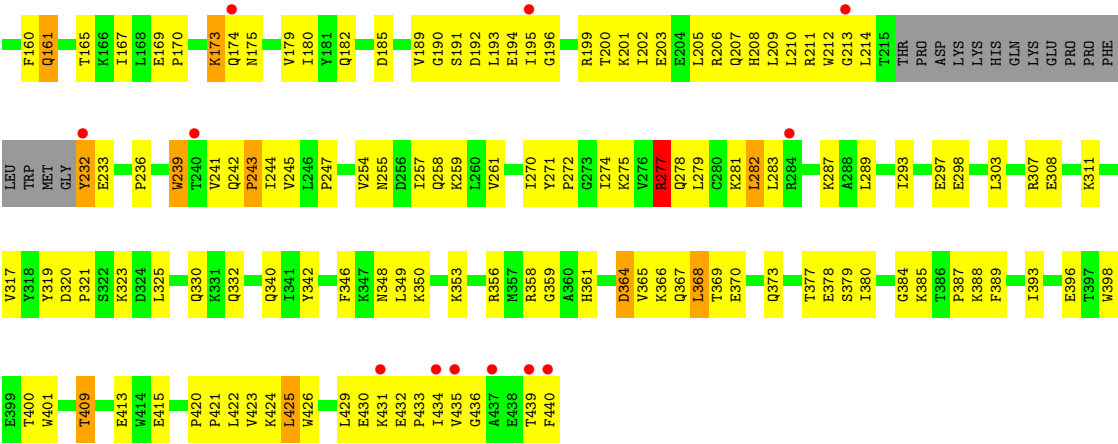
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN)



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.80Å 109.50Å 71.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.50) 92.7 (29.38-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.315 0.222 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 68.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CSD, 612

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	0.41	0/4503	0.65	0/6118
2	B	0.40	0/3533	0.63	0/4797
All	All	0.41	0/8036	0.64	0/10915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4396	0	4442	256	0
2	B	3437	0	3466	205	0
3	A	22	0	26	4	0
4	A	95	0	0	10	0
4	B	47	0	0	7	0
All	All	7997	0	7934	449	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 28.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.36	1.06
1:A:239:TRP:CE2	1:A:316:GLY:HA3	1.97	0.99
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.48	0.96
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.63	0.96
2:B:125:ARG:HE	2:B:147:ASN:HA	1.30	0.95
1:A:332:GLN:HE22	1:A:353:LYS:HE3	1.28	0.94
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.09	0.94
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.50	0.94
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.03	0.93
1:A:280:CSD:C	1:A:281:LYS:N	2.33	0.90
1:A:57:ASN:HD22	1:A:143:ARG:NH2	1.69	0.90
1:A:102:LYS:HB2	1:A:102:LYS:NZ	1.90	0.87
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.39	0.87
2:B:169:GLU:HG3	2:B:173:LYS:HD3	1.56	0.86
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.10	0.86
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.54	0.86
2:B:78:ARG:O	2:B:82:LYS:HG3	1.76	0.86
1:A:358:ARG:H	1:A:358:ARG:HD3	1.43	0.84
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.60	0.84
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.24	0.84
2:B:245:VAL:HG21	2:B:431:LYS:HD3	1.58	0.83
1:A:57:ASN:ND2	1:A:143:ARG:HH21	1.78	0.82
2:B:63:ILE:HD11	2:B:74:LEU:HD23	1.62	0.81
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.61	0.81
2:B:84:THR:HB	2:B:154:LYS:HE2	1.61	0.81
2:B:366:LYS:O	2:B:370:GLU:HG3	1.82	0.80
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.17	0.79
2:B:161:GLN:HE22	2:B:182:GLN:HE22	1.27	0.79
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.81	0.77
2:B:409:THR:HG21	4:B:1084:HOH:O	1.83	0.77
2:B:161:GLN:HE22	2:B:182:GLN:NE2	1.83	0.77
1:A:332:GLN:NE2	1:A:353:LYS:HE3	1.99	0.77
2:B:257:ILE:O	2:B:261:VAL:HG23	1.84	0.76
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.16	0.75
1:A:515:SER:CB	1:A:518:VAL:HG23	2.16	0.75
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.68	0.75
2:B:180:ILE:HG13	2:B:189:VAL:HG22	1.66	0.75
1:A:4:PRO:HA	4:A:1003:HOH:O	1.87	0.74
1:A:308:GLU:HG2	4:A:1132:HOH:O	1.87	0.73
1:A:335:GLY:HA3	1:A:356:ARG:HD2	1.70	0.73
2:B:365:VAL:O	2:B:369:THR:HG23	1.88	0.73
1:A:17:ASP:O	1:A:83:ARG:HD3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:HB2	1:A:92:LEU:HD23	1.70	0.73
2:B:373:GLN:O	2:B:377:THR:HG23	1.88	0.73
2:B:208:HIS:O	2:B:211:ARG:HB3	1.89	0.72
2:B:194:GLU:HG3	4:B:1147:HOH:O	1.89	0.72
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.71	0.72
1:A:502:ALA:O	1:A:506:ILE:HG13	1.90	0.72
1:A:484:LEU:HD23	1:A:487:GLN:NE2	2.05	0.72
2:B:73:LYS:HB3	2:B:73:LYS:HZ2	1.55	0.71
1:A:279:LEU:HG	1:A:302:GLU:OE1	1.89	0.71
2:B:79:GLU:O	2:B:83:ARG:HG3	1.90	0.71
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.26	0.71
1:A:475:GLN:HG3	1:A:476:LYS:N	2.04	0.71
1:A:2:ILE:HG23	1:A:3:SER:N	2.05	0.70
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.74	0.70
1:A:102:LYS:HB2	1:A:102:LYS:HZ2	1.55	0.70
1:A:255:ASN:ND2	1:A:289:LEU:HD12	2.07	0.70
1:A:399:GLU:O	1:A:403:THR:HB	1.92	0.70
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.92	0.69
1:A:102:LYS:HZ3	1:A:237:ASP:HA	1.57	0.69
2:B:63:ILE:CD1	2:B:74:LEU:HD23	2.22	0.69
1:A:99:GLY:HA3	2:B:136:ASN:ND2	2.06	0.69
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.75	0.69
2:B:325:LEU:HD22	2:B:385:LYS:HD2	1.71	0.69
1:A:23:GLN:HG2	1:A:133:PRO:HD3	1.74	0.69
1:A:332:GLN:HE22	1:A:353:LYS:CE	2.04	0.69
2:B:379:SER:CB	2:B:387:PRO:HD3	2.23	0.69
2:B:421:PRO:O	2:B:425:LEU:HD22	1.94	0.68
1:A:99:GLY:HA3	2:B:136:ASN:HD22	1.59	0.68
2:B:173:LYS:HD2	2:B:173:LYS:N	2.09	0.67
2:B:242:GLN:HG3	2:B:243:PRO:HD2	1.75	0.67
2:B:275:LYS:HB3	2:B:277:ARG:HG2	1.75	0.67
2:B:270:ILE:O	2:B:272:PRO:HD3	1.94	0.67
1:A:20:LYS:NZ	1:A:20:LYS:HB3	2.10	0.67
1:A:255:ASN:HD21	1:A:289:LEU:HD12	1.60	0.67
1:A:344:GLU:HG3	1:A:347:LYS:HD3	1.75	0.67
1:A:208:HIS:O	1:A:211:ARG:HB2	1.93	0.67
1:A:257:ILE:O	1:A:261:VAL:HG23	1.94	0.66
1:A:246:LEU:O	1:A:307:ARG:NH1	2.28	0.66
1:A:32:LYS:HE3	1:A:32:LYS:HA	1.79	0.65
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.77	0.65
1:A:104:LYS:HD2	1:A:192:ASP:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:GLU:HG3	2:B:433:PRO:HD2	1.78	0.65
1:A:94:ILE:H	1:A:94:ILE:CD1	2.09	0.65
1:A:102:LYS:HZ2	1:A:102:LYS:CB	2.09	0.64
1:A:64:LYS:HG3	1:A:71:TRP:CZ3	2.33	0.63
1:A:255:ASN:O	1:A:259:LYS:HG2	1.98	0.63
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.08	0.63
1:A:360:ALA:O	1:A:513:SER:HB2	1.97	0.63
2:B:432:GLU:CG	2:B:433:PRO:HD2	2.28	0.63
1:A:113:ASP:HB3	4:A:1127:HOH:O	1.99	0.63
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.81	0.62
2:B:125:ARG:NE	2:B:147:ASN:HA	2.09	0.62
2:B:388:LYS:HZ3	2:B:415:GLU:HG2	1.65	0.62
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.39	0.61
1:A:102:LYS:NZ	1:A:102:LYS:CB	2.61	0.61
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.82	0.61
1:A:301:LEU:O	1:A:304:ALA:HB3	2.00	0.61
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.82	0.61
2:B:195:ILE:HG23	2:B:196:GLY:N	2.14	0.61
2:B:161:GLN:NE2	2:B:182:GLN:HE22	1.98	0.61
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.81	0.61
2:B:35:VAL:O	2:B:39:THR:HG23	2.01	0.61
2:B:205:LEU:O	2:B:208:HIS:HB3	2.00	0.61
2:B:388:LYS:NZ	2:B:415:GLU:HG2	2.15	0.60
1:A:317:VAL:HG21	1:A:347:LYS:HB3	1.83	0.60
2:B:31:ILE:O	2:B:35:VAL:HG23	2.01	0.60
1:A:229:TRP:CD1	1:A:230:MET:HG2	2.36	0.60
2:B:243:PRO:HD2	2:B:431:LYS:HB3	1.84	0.60
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.84	0.60
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.16	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
1:A:317:VAL:HG12	1:A:318:TYR:N	2.17	0.60
2:B:303:LEU:HD23	2:B:303:LEU:O	2.02	0.60
1:A:109:LEU:HD11	1:A:206:ARG:HH12	1.67	0.60
2:B:207:GLN:O	2:B:210:LEU:HB3	2.02	0.60
1:A:478:GLU:O	1:A:481:ALA:HB3	2.02	0.59
2:B:122:GLU:HA	2:B:125:ARG:NH1	2.18	0.59
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.38	0.59
1:A:112:GLY:O	1:A:114:ALA:N	2.36	0.59
1:A:500:GLN:HE21	1:A:500:GLN:HA	1.65	0.59
1:A:80:LEU:O	1:A:83:ARG:N	2.36	0.59
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HG23	1:A:3:SER:H	1.68	0.59
1:A:492:GLU:HA	1:A:530:LYS:O	2.03	0.59
1:A:120:LEU:HD22	1:A:121:ASP:H	1.68	0.59
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.67	0.58
1:A:122:GLU:H	1:A:122:GLU:CD	2.05	0.58
2:B:73:LYS:HB3	2:B:73:LYS:NZ	2.16	0.58
2:B:160:PHE:O	2:B:160:PHE:CD1	2.57	0.58
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.86	0.57
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.85	0.57
1:A:164:MET:O	1:A:168:LEU:HG	2.04	0.57
2:B:151:GLN:HG3	4:B:1083:HOH:O	2.04	0.57
1:A:109:LEU:HD11	1:A:206:ARG:NH1	2.20	0.57
1:A:279:LEU:O	1:A:282:LEU:HB2	2.04	0.57
1:A:28:GLU:O	1:A:32:LYS:HG2	2.04	0.57
1:A:94:ILE:H	1:A:94:ILE:HD13	1.68	0.57
1:A:260:LEU:O	1:A:264:LEU:HD23	2.04	0.57
2:B:101:LYS:O	2:B:236:PRO:HB2	2.05	0.57
2:B:175:ASN:HD21	2:B:201:LYS:HZ1	1.50	0.57
2:B:242:GLN:HG2	2:B:431:LYS:O	2.05	0.57
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.40	0.57
1:A:249:LYS:HE2	1:A:256:ASP:OD2	2.04	0.56
1:A:312:GLU:OE2	1:A:312:GLU:HA	2.06	0.56
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.06	0.56
2:B:161:GLN:O	2:B:165:THR:HG23	2.05	0.56
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.88	0.56
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.87	0.56
1:A:500:GLN:HA	1:A:500:GLN:NE2	2.21	0.56
2:B:369:THR:O	2:B:373:GLN:HG3	2.06	0.56
2:B:203:GLU:O	2:B:206:ARG:HB3	2.05	0.56
2:B:422:LEU:HA	2:B:425:LEU:HD23	1.88	0.56
1:A:102:LYS:HB2	1:A:102:LYS:HZ1	1.71	0.56
1:A:112:GLY:C	1:A:114:ALA:H	2.09	0.55
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.88	0.55
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.17	0.55
1:A:360:ALA:CA	1:A:514:GLU:HG2	2.29	0.55
2:B:353:LYS:NZ	2:B:430:GLU:HB3	2.21	0.55
1:A:54:ASN:HB3	1:A:143:ARG:NH1	2.22	0.55
1:A:275:LYS:HD2	4:A:1045:HOH:O	2.06	0.55
2:B:88:TRP:HZ3	2:B:93:GLY:N	2.05	0.55
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.32	0.55
1:A:57:ASN:HA	1:A:129:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.35	0.54
1:A:237:ASP:HB3	4:A:1033:HOH:O	2.06	0.54
1:A:307:ARG:O	1:A:311:LYS:HG3	2.07	0.54
1:A:90:VAL:HB	1:A:158:ALA:HA	1.90	0.54
1:A:27:THR:O	1:A:31:ILE:HG13	2.07	0.54
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.72	0.54
1:A:376:THR:O	1:A:380:ILE:HG12	2.06	0.54
1:A:170:PRO:O	1:A:174:GLN:HG3	2.08	0.54
1:A:64:LYS:H	1:A:64:LYS:HD2	1.72	0.54
1:A:516:GLU:HA	1:A:519:ASN:ND2	2.23	0.54
2:B:245:VAL:HG23	2:B:431:LYS:HB2	1.90	0.54
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.89	0.54
2:B:56:TYR:O	2:B:57:ASN:HB2	2.08	0.54
2:B:97:PRO:HG2	2:B:100:LEU:HB2	1.88	0.54
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.20	0.54
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.90	0.53
2:B:170:PRO:O	2:B:174:GLN:HB2	2.08	0.53
1:A:116:PHE:CE2	1:A:151:GLN:HG3	2.42	0.53
1:A:235:HIS:HB2	1:A:238:LYS:O	2.07	0.53
2:B:106:VAL:HG22	2:B:190:GLY:HA3	1.89	0.53
2:B:379:SER:OG	2:B:387:PRO:HD3	2.08	0.53
2:B:118:VAL:HB	2:B:149:LEU:HG	1.90	0.53
1:A:326:ILE:HD12	1:A:326:ILE:N	2.23	0.53
1:A:355:ALA:O	1:A:356:ARG:C	2.47	0.53
1:A:408:ALA:HA	2:B:364:ASP:OD1	2.09	0.53
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.91	0.52
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.44	0.52
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.39	0.52
2:B:122:GLU:HA	2:B:125:ARG:HH11	1.73	0.52
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.44	0.52
2:B:185:ASP:HB3	4:B:1084:HOH:O	2.09	0.52
2:B:173:LYS:HD2	2:B:173:LYS:H	1.75	0.52
1:A:102:LYS:NZ	1:A:237:ASP:HA	2.23	0.52
1:A:231:GLY:C	1:A:242:GLN:HG3	2.30	0.52
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.42	0.52
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.44	0.52
2:B:114:ALA:CA	2:B:214:LEU:HD21	2.40	0.52
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.39	0.52
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.44	0.52
2:B:287:LYS:HD2	2:B:293:ILE:HD11	1.92	0.52
1:A:476:LYS:O	1:A:480:GLN:N	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TRP:CB	1:A:61:PHE:HE1	2.22	0.51
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.41	0.51
2:B:13:LYS:NZ	2:B:82:LYS:O	2.42	0.51
2:B:433:PRO:HB2	2:B:436:GLY:HA2	1.93	0.51
1:A:483:TYR:O	1:A:487:GLN:HG3	2.10	0.51
1:A:500:GLN:HE21	1:A:500:GLN:CA	2.23	0.51
1:A:108:VAL:CG1	1:A:223:LYS:HB2	2.38	0.51
1:A:58:THR:CG2	1:A:76:ASP:O	2.58	0.51
1:A:358:ARG:HD3	1:A:358:ARG:N	2.21	0.51
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.34	0.51
2:B:195:ILE:HG23	2:B:196:GLY:H	1.76	0.51
2:B:287:LYS:CD	2:B:293:ILE:HD11	2.41	0.51
1:A:314:VAL:HA	4:A:1050:HOH:O	2.11	0.51
1:A:409:THR:O	2:B:364:ASP:HB2	2.11	0.50
1:A:516:GLU:O	1:A:519:ASN:HB2	2.11	0.50
2:B:64:LYS:HE2	2:B:71:TRP:CE2	2.46	0.50
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.11	0.50
1:A:3:SER:HB3	1:A:5:ILE:CG1	2.38	0.50
1:A:254:VAL:HB	1:A:289:LEU:O	2.11	0.50
2:B:114:ALA:HB2	2:B:214:LEU:HD21	1.92	0.50
2:B:116:PHE:CD2	2:B:117:SER:N	2.79	0.50
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.46	0.50
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.94	0.50
1:A:54:ASN:HB3	1:A:143:ARG:HH12	1.75	0.50
1:A:332:GLN:O	1:A:332:GLN:HG2	2.12	0.50
1:A:536:VAL:HG11	2:B:258:GLN:NE2	2.26	0.50
2:B:161:GLN:NE2	2:B:182:GLN:NE2	2.55	0.50
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.27	0.50
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.92	0.50
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.93	0.50
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.47	0.50
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.47	0.50
2:B:332:GLN:HE22	2:B:424:LYS:HD3	1.76	0.50
1:A:317:VAL:CG1	1:A:318:TYR:N	2.75	0.49
2:B:209:LEU:HD12	2:B:214:LEU:HD12	1.93	0.49
1:A:135:ILE:O	1:A:138:GLU:HG3	2.13	0.49
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.12	0.49
1:A:96:HIS:HB2	4:A:1017:HOH:O	2.12	0.49
1:A:31:ILE:O	1:A:35:VAL:HG23	2.12	0.49
1:A:167:ILE:O	1:A:170:PRO:HD2	2.12	0.49
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HG3	1:A:476:LYS:H	1.73	0.49
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.12	0.49
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.11	0.49
2:B:425:LEU:O	2:B:429:LEU:HD13	2.12	0.49
1:A:498:ASP:HA	1:A:536:VAL:O	2.13	0.49
2:B:97:PRO:O	2:B:99:GLY:N	2.46	0.49
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.13	0.49
2:B:232:TYR:HD1	2:B:233:GLU:N	2.11	0.49
2:B:58:THR:HG23	2:B:76:ASP:O	2.13	0.48
2:B:281:LYS:C	2:B:283:LEU:H	2.15	0.48
1:A:282:LEU:HD12	1:A:293:ILE:HG22	1.95	0.48
1:A:289:LEU:H	1:A:289:LEU:HD22	1.79	0.48
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.13	0.48
1:A:112:GLY:C	1:A:114:ALA:N	2.67	0.48
2:B:380:ILE:O	2:B:384:GLY:N	2.42	0.48
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.13	0.48
1:A:64:LYS:HD2	1:A:64:LYS:N	2.26	0.48
2:B:43:LYS:HA	2:B:43:LYS:HD3	1.58	0.48
2:B:434:ILE:HG22	2:B:435:VAL:HG13	1.96	0.48
1:A:363:ASN:HA	1:A:511:ASP:CG	2.33	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.14	0.48
1:A:436:GLY:O	1:A:461:ARG:NH2	2.47	0.48
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.95	0.48
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.96	0.48
2:B:98:ALA:HA	2:B:101:LYS:NZ	2.29	0.48
2:B:206:ARG:NH1	2:B:206:ARG:HG2	2.28	0.48
2:B:308:GLU:OE1	2:B:311:LYS:HD2	2.14	0.48
2:B:433:PRO:CB	2:B:436:GLY:HA2	2.43	0.48
1:A:234:LEU:N	1:A:234:LEU:HD22	2.28	0.47
2:B:53:GLU:OE1	2:B:53:GLU:N	2.40	0.47
1:A:95:PRO:CA	2:B:136:ASN:OD1	2.60	0.47
1:A:383:TRP:O	1:A:385:LYS:HG2	2.14	0.47
2:B:50:ILE:HG21	2:B:145:GLN:CB	2.44	0.47
2:B:167:ILE:O	2:B:208:HIS:NE2	2.47	0.47
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.46	0.47
2:B:317:VAL:HG11	2:B:348:ASN:O	2.14	0.47
1:A:33:ALA:O	1:A:36:GLU:HB3	2.15	0.47
2:B:205:LEU:CD2	2:B:209:LEU:HD23	2.45	0.47
1:A:116:PHE:HE1	1:A:146:TYR:HE1	1.63	0.47
1:A:356:ARG:NH1	1:A:357:MET:O	2.48	0.47
3:A:999:612:C6	3:A:999:612:HIA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD12	1:A:293:ILE:CG2	2.45	0.47
2:B:111:VAL:HG23	2:B:111:VAL:O	2.13	0.47
2:B:94:ILE:HD11	2:B:182:GLN:H	1.80	0.47
1:A:23:GLN:CG	1:A:133:PRO:HD3	2.44	0.46
1:A:454:LYS:HA	1:A:467:VAL:O	2.15	0.46
2:B:278:GLN:HA	2:B:278:GLN:NE2	2.30	0.46
1:A:116:PHE:HE1	1:A:146:TYR:CE1	2.32	0.46
2:B:64:LYS:HE2	2:B:71:TRP:CZ2	2.50	0.46
1:A:58:THR:HG23	1:A:76:ASP:O	2.16	0.46
1:A:480:GLN:HE21	1:A:480:GLN:CA	2.27	0.46
1:A:84:THR:HG22	1:A:85:GLN:O	2.16	0.46
2:B:5:ILE:HB	2:B:6:GLU:H	1.61	0.46
1:A:1:PRO:HA	4:A:1002:HOH:O	2.14	0.46
1:A:64:LYS:H	1:A:64:LYS:CD	2.28	0.46
2:B:137:ASN:N	2:B:137:ASN:HD22	2.13	0.46
2:B:319:TYR:OH	2:B:385:LYS:HE3	2.15	0.46
1:A:171:PHE:CE1	1:A:205:LEU:HG	2.51	0.46
1:A:280:CSD:O	1:A:281:LYS:N	2.47	0.46
2:B:167:ILE:HG22	2:B:212:TRP:CH2	2.51	0.46
1:A:79:GLU:O	1:A:82:LYS:HB3	2.16	0.46
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.98	0.46
2:B:46:LYS:HE2	2:B:116:PHE:HD1	1.80	0.46
2:B:74:LEU:HD21	2:B:409:THR:HA	1.96	0.46
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.51	0.46
1:A:344:GLU:CG	1:A:347:LYS:HD3	2.45	0.46
1:A:77:PHE:CE1	1:A:150:PRO:HB2	2.50	0.45
2:B:255:ASN:OD1	2:B:259:LYS:HE3	2.16	0.45
1:A:20:LYS:HB3	1:A:20:LYS:HZ3	1.81	0.45
2:B:65:LYS:HE3	2:B:72:ARG:HD2	1.98	0.45
1:A:339:TYR:CE2	1:A:352:GLY:HA3	2.51	0.45
2:B:52:PRO:HD2	2:B:53:GLU:OE1	2.16	0.45
1:A:132:ILE:O	1:A:141:GLY:HA3	2.16	0.45
2:B:103:LYS:HD2	2:B:191:SER:HA	1.99	0.45
2:B:279:LEU:O	2:B:282:LEU:HD12	2.17	0.45
2:B:173:LYS:HE3	4:B:1090:HOH:O	2.17	0.45
2:B:319:TYR:CE1	2:B:321:PRO:HG3	2.52	0.45
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.47	0.45
2:B:156:SER:HB2	2:B:157:PRO:CD	2.47	0.45
1:A:241:VAL:HG21	1:A:270:ILE:HG21	1.97	0.45
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.47	0.45
2:B:205:LEU:C	2:B:205:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.48	0.45
1:A:33:ALA:O	1:A:37:ILE:HG13	2.16	0.44
2:B:195:ILE:CG2	2:B:196:GLY:N	2.80	0.44
1:A:40:GLU:O	1:A:44:GLU:HG3	2.17	0.44
1:A:90:VAL:HG22	1:A:90:VAL:O	2.18	0.44
1:A:153:TRP:CH2	1:A:155:GLY:HA3	2.51	0.44
1:A:360:ALA:O	1:A:361:HIS:HB3	2.17	0.44
1:A:399:GLU:OE2	1:A:402:TRP:HZ3	2.01	0.44
1:A:480:GLN:CA	1:A:480:GLN:NE2	2.80	0.44
1:A:408:ALA:HB3	2:B:393:ILE:CG1	2.48	0.44
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.99	0.44
2:B:77:PHE:O	2:B:78:ARG:C	2.55	0.44
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.00	0.44
2:B:114:ALA:N	2:B:214:LEU:HD21	2.32	0.44
1:A:94:ILE:HD13	1:A:94:ILE:N	2.28	0.44
1:A:111:VAL:O	1:A:114:ALA:HB3	2.18	0.44
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.00	0.44
2:B:303:LEU:HD22	2:B:307:ARG:HE	1.82	0.44
1:A:150:PRO:HG2	1:A:153:TRP:HB2	2.00	0.44
3:A:999:612:HHB	3:A:999:612:S	2.57	0.44
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.52	0.44
2:B:297:GLU:HA	2:B:297:GLU:OE1	2.17	0.44
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.53	0.43
2:B:7:THR:CG2	2:B:119:PRO:HB2	2.48	0.43
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.99	0.43
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.53	0.43
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.00	0.43
2:B:74:LEU:HD13	2:B:75:VAL:N	2.33	0.43
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.83	0.43
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.99	0.43
1:A:489:SER:OG	1:A:493:VAL:HG21	2.17	0.43
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.54	0.43
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.53	0.43
1:A:524:GLN:O	1:A:528:LYS:HG2	2.19	0.43
2:B:97:PRO:C	2:B:99:GLY:N	2.72	0.43
2:B:175:ASN:HD21	2:B:201:LYS:HE3	1.82	0.43
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.59	0.43
1:A:59:PRO:HB2	1:A:61:PHE:CZ	2.54	0.43
1:A:419:THR:HG22	4:A:1061:HOH:O	2.19	0.43
1:A:428:GLN:O	1:A:429:LEU:C	2.57	0.43
2:B:65:LYS:CG	2:B:72:ARG:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.34	0.43
2:B:275:LYS:HB3	2:B:277:ARG:CG	2.45	0.43
2:B:325:LEU:HD12	2:B:325:LEU:HA	1.79	0.43
2:B:368:LEU:HD13	2:B:398:TRP:CZ3	2.53	0.43
1:A:465:LYS:HG2	1:A:466:VAL:N	2.34	0.42
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.49	0.42
1:A:280:CSD:O	1:A:282:LEU:N	2.52	0.42
2:B:271:TYR:HB2	2:B:274:ILE:HD12	2.00	0.42
2:B:433:PRO:CG	2:B:436:GLY:HA2	2.49	0.42
2:B:439:THR:O	2:B:440:PHE:OXT	2.36	0.42
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.84	0.42
1:A:137:ASN:O	1:A:137:ASN:CG	2.58	0.42
1:A:302:GLU:HA	1:A:305:GLU:OE1	2.19	0.42
2:B:102:LYS:O	2:B:103:LYS:C	2.57	0.42
1:A:8:VAL:HG13	1:A:9:PRO:HD2	2.01	0.42
1:A:32:LYS:HE3	1:A:32:LYS:CA	2.46	0.42
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.54	0.42
2:B:137:ASN:N	2:B:137:ASN:ND2	2.67	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.54	0.42
3:A:999:612:HIA	3:A:999:612:H6	2.01	0.42
2:B:241:VAL:HG22	2:B:350:LYS:HG3	2.01	0.42
2:B:342:TYR:HB3	2:B:348:ASN:HA	2.01	0.42
2:B:353:LYS:HE3	2:B:353:LYS:HB2	1.69	0.42
2:B:413:GLU:HA	2:B:413:GLU:OE2	2.19	0.42
1:A:85:GLN:O	1:A:154:LYS:NZ	2.52	0.42
1:A:381:VAL:HG22	2:B:25:PRO:HB3	2.01	0.42
1:A:119:PRO:HA	1:A:148:VAL:HA	2.02	0.42
1:A:442:VAL:HG13	1:A:495:ILE:HG23	2.02	0.42
2:B:195:ILE:HG22	4:B:1147:HOH:O	2.20	0.42
2:B:199:ARG:O	2:B:202:ILE:HB	2.20	0.42
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.41
1:A:14:PRO:HD3	4:A:1007:HOH:O	2.18	0.41
1:A:164:MET:HE1	1:A:214:LEU:HD13	2.00	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41
1:A:93:GLY:O	2:B:137:ASN:OD1	2.39	0.41
2:B:103:LYS:HG3	2:B:190:GLY:O	2.20	0.41
1:A:33:ALA:HB1	1:A:71:TRP:HB3	2.02	0.41
1:A:312:GLU:CD	1:A:313:PRO:HD2	2.41	0.41
1:A:328:GLU:O	1:A:339:TYR:HA	2.19	0.41
2:B:66:LYS:HD3	4:B:1118:HOH:O	2.20	0.41
2:B:212:TRP:CD1	2:B:212:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:413:GLU:C	2.59	0.41
1:A:64:LYS:HD2	1:A:64:LYS:O	2.21	0.41
1:A:228:LEU:HA	1:A:232:TYR:O	2.21	0.41
2:B:396:GLU:H	2:B:396:GLU:CD	2.24	0.41
1:A:49:LYS:HA	1:A:144:TYR:CD2	2.56	0.41
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.82	0.41
1:A:89:GLU:O	1:A:89:GLU:OE1	2.39	0.41
1:A:104:LYS:HD2	1:A:192:ASP:C	2.40	0.41
1:A:129:ALA:HA	1:A:144:TYR:O	2.21	0.41
1:A:205:LEU:O	1:A:209:LEU:HG	2.20	0.41
1:A:295:LEU:HD22	1:A:299:ALA:HB1	2.02	0.41
2:B:116:PHE:O	2:B:148:VAL:HG11	2.21	0.41
2:B:195:ILE:O	2:B:199:ARG:HG3	2.21	0.41
2:B:213:GLY:O	2:B:214:LEU:HG	2.19	0.41
2:B:303:LEU:HD22	2:B:307:ARG:NE	2.35	0.41
1:A:20:LYS:HB3	1:A:20:LYS:HZ2	1.82	0.41
1:A:332:GLN:HE21	1:A:332:GLN:HB3	1.67	0.41
1:A:361:HIS:HA	1:A:512:GLN:O	2.21	0.41
2:B:51:GLY:HA3	2:B:53:GLU:OE1	2.21	0.41
2:B:98:ALA:HA	2:B:101:LYS:HZ3	1.86	0.41
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.03	0.41
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.85	0.40
1:A:116:PHE:CE1	1:A:146:TYR:HE1	2.39	0.40
1:A:28:GLU:HG3	1:A:29:GLU:N	2.35	0.40
1:A:188:TYR:CD2	3:A:999:612:H2	2.56	0.40
1:A:386:THR:HA	1:A:387:PRO:HD3	1.79	0.40
1:A:388:LYS:HG3	1:A:413:GLU:OE2	2.21	0.40
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.03	0.40
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.22	0.40
1:A:50:ILE:CG2	1:A:145:GLN:HG2	2.51	0.40
1:A:111:VAL:O	1:A:114:ALA:CB	2.69	0.40
2:B:308:GLU:O	2:B:311:LYS:HB2	2.21	0.40
1:A:135:ILE:HD12	1:A:135:ILE:N	2.36	0.40
1:A:519:ASN:O	1:A:523:GLU:HG2	2.22	0.40
1:A:93:GLY:C	2:B:137:ASN:OD1	2.60	0.40
1:A:111:VAL:HG22	1:A:185:ASP:O	2.22	0.40
1:A:377:THR:O	1:A:381:VAL:HG23	2.21	0.40
1:A:480:GLN:HE21	1:A:480:GLN:C	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/560 (95%)	473 (89%)	42 (8%)	16 (3%)	4	6
2	B	410/440 (93%)	357 (87%)	45 (11%)	8 (2%)	7	12
All	All	941/1000 (94%)	830 (88%)	87 (9%)	24 (3%)	5	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LEU
1	A	91	GLN
1	A	112	GLY
1	A	113	ASP
1	A	125	ARG
1	A	135	ILE
1	A	136	ASN
1	A	137	ASN
1	A	217	PRO
1	A	356	ARG
1	A	361	HIS
2	B	98	ALA
2	B	277	ARG
2	B	358	ARG
1	A	2	ILE
1	A	85	GLN
2	B	103	LYS
2	B	239	TRP
1	A	14	PRO
1	A	215	THR
2	B	282	LEU
2	B	247	PRO
1	A	345	PRO
1	A	133	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	481/499 (96%)	448 (93%)	33 (7%)	15	30
2	B	377/400 (94%)	357 (95%)	20 (5%)	22	43
All	All	858/899 (95%)	805 (94%)	53 (6%)	18	35

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	20	LYS
1	A	21	VAL
1	A	32	LYS
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	73	LYS
1	A	89	GLU
1	A	94	ILE
1	A	102	LYS
1	A	109	LEU
1	A	120	LEU
1	A	149	LEU
1	A	151	GLN
1	A	173	LYS
1	A	205	LEU
1	A	340	GLN
1	A	357	MET
1	A	358	ARG
1	A	361	HIS
1	A	368	LEU
1	A	402	TRP
1	A	403	THR
1	A	448	ARG
1	A	475	GLN
1	A	477	THR

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	491	LEU
1	A	496	VAL
1	A	501	TYR
1	A	514	GLU
1	A	517	LEU
2	B	5	ILE
2	B	6	GLU
2	B	32	LYS
2	B	40	GLU
2	B	41	MET
2	B	74	LEU
2	B	86	ASP
2	B	116	PHE
2	B	126	LYS
2	B	161	GLN
2	B	173	LYS
2	B	192	ASP
2	B	200	THR
2	B	232	TYR
2	B	243	PRO
2	B	277	ARG
2	B	364	ASP
2	B	368	LEU
2	B	409	THR
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	151	GLN
1	A	161	GLN
1	A	174	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	330	GLN
1	A	332	GLN
1	A	336	GLN
1	A	361	HIS
1	A	475	GLN

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	487	GLN
1	A	500	GLN
1	A	512	GLN
1	A	519	ASN
2	B	57	ASN
2	B	151	GLN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	394	GLN
2	B	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
1	CSD	A	280	1	3,7,8	0.61	0	1,8,10	5.54	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	5.54	116.09	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	612	A	999	-	22,23,23	1.75	1 (4%)	24,31,31	0.67	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	612	A	999	-	-	1/10/20/20	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	612	C7-S	7.34	1.86	1.75

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

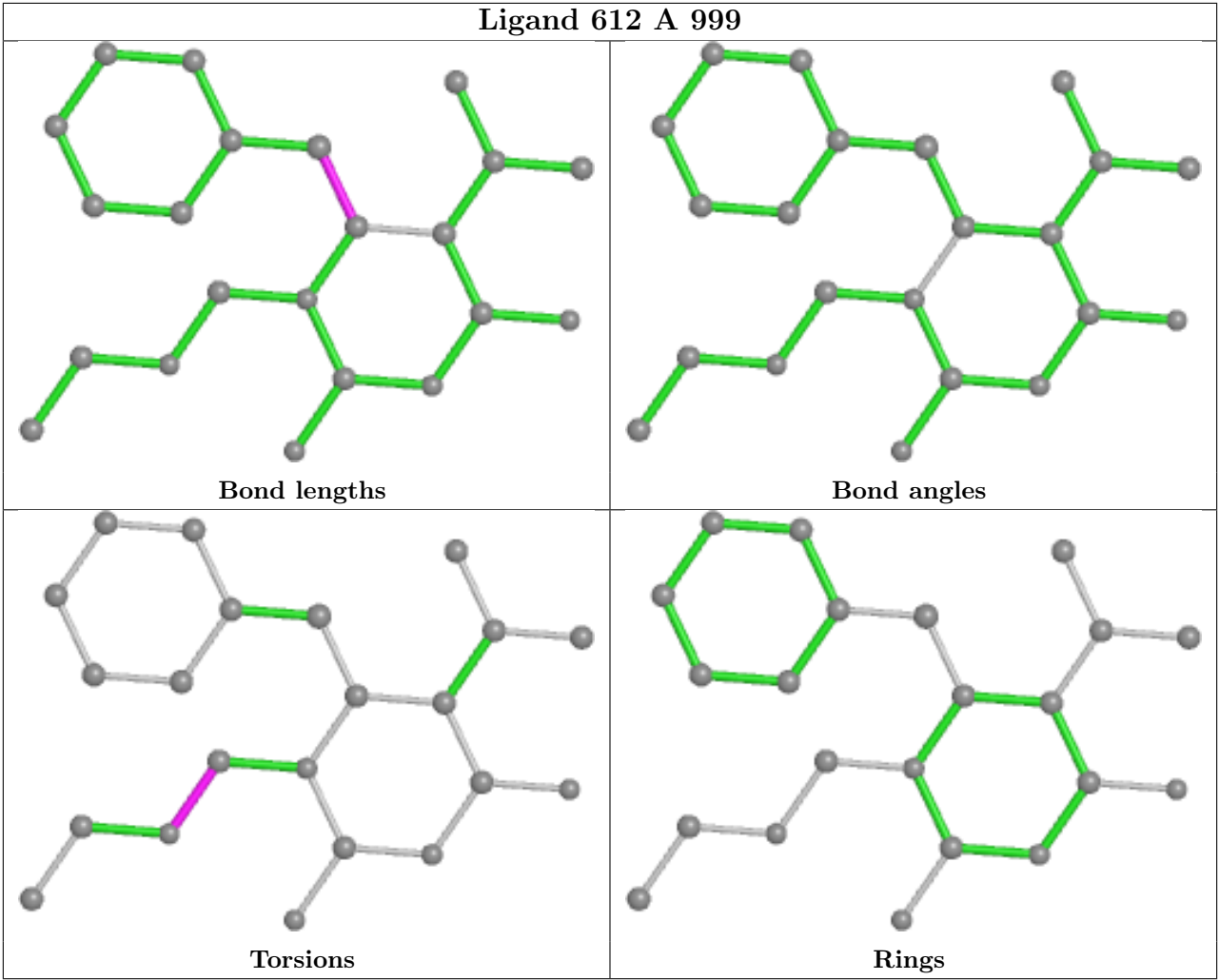
Mol	Chain	Res	Type	Atoms
3	A	999	612	N8-CA-OB-CC

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	612	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	280:CSD	C	281:LYS	N	2.33

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	536/560 (95%)	-0.01	20 (3%)	41 45	9, 42, 85, 120	0
2	B	416/440 (94%)	0.19	23 (5%)	25 26	13, 44, 94, 126	0
All	All	952/1000 (95%)	0.08	43 (4%)	33 36	9, 43, 90, 126	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	7.8
2	B	232	TYR	6.9
2	B	67	ASP	6.8
2	B	213	GLY	6.4
1	A	69	THR	5.5
2	B	65	LYS	4.8
1	A	115	TYR	4.7
2	B	104	LYS	4.6
1	A	448	ARG	4.6
2	B	439	THR	4.4
2	B	68	SER	3.8
2	B	66	LYS	3.8
1	A	116	PHE	3.7
2	B	94	ILE	3.6
1	A	358	ARG	3.5
1	A	92	LEU	3.5
2	B	69	THR	3.4
2	B	435	VAL	3.4
2	B	195	ILE	3.2
2	B	434	ILE	3.2
2	B	440	PHE	3.2
1	A	71	TRP	3.1
1	A	66	LYS	3.0
1	A	90	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	116	PHE	2.8
1	A	64	LYS	2.7
2	B	284	ARG	2.6
1	A	245	VAL	2.6
1	A	24	TRP	2.4
2	B	88	TRP	2.4
1	A	65	LYS	2.4
1	A	43	LYS	2.4
2	B	174	GLN	2.3
1	A	2	ILE	2.3
2	B	5	ILE	2.2
2	B	70	LYS	2.2
1	A	221	HIS	2.2
1	A	139	THR	2.2
2	B	437	ALA	2.1
1	A	136	ASN	2.1
1	A	357	MET	2.1
2	B	240	THR	2.0
2	B	431	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSD	A	280	8/9	0.95	0.13	13,26,47,48	0

## 6.3 Carbohydrates [i](#)

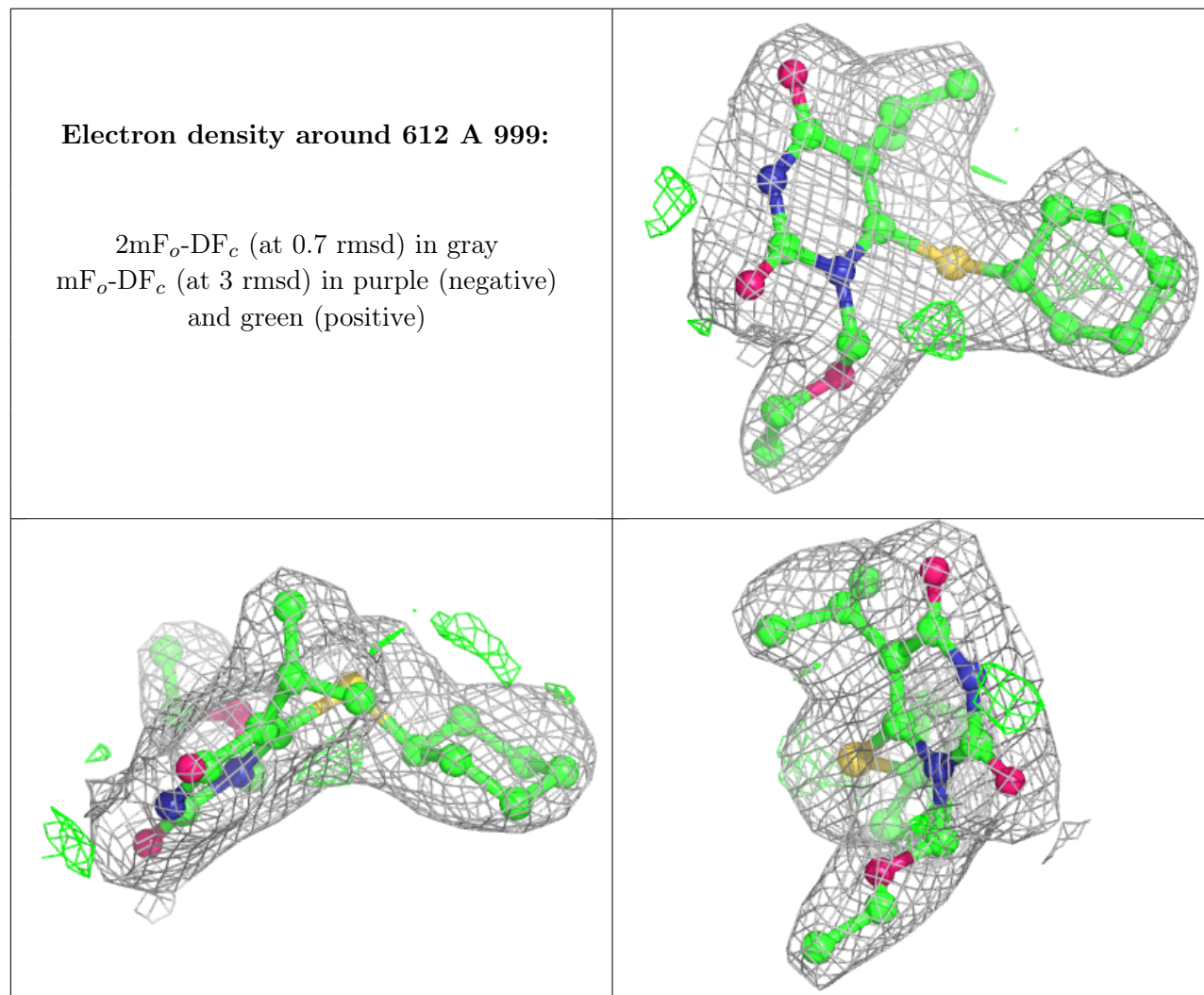
There are no monosaccharides in this entry.

## 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<sup>th</sup> 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	612	A	999	22/22	0.94	0.16	10,21,32,34	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.