



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 2YKM / pdb_00002ykm
Title : Crystal structure of HIV-1 Reverse Transcriptase (RT) in complex with a D ifluoromethylbenzoxazole (DFMB) Pyrimidine Thioether derivative, a non-nucleoside RT inhibitor (NNRTI)
Authors : Boyer, J.; Arnoult, E.; Medebielle, M.; Guillemont, J.; Unge, T.; Unge, J.; Jochmans, D.
Deposited on : 2011-05-28
Resolution : 2.90 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](#) ①) 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

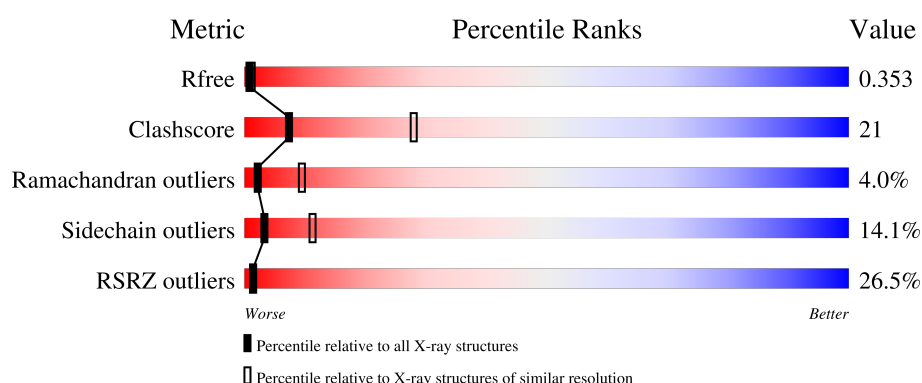
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	562	35% 55% 36% 7% ..
2	B	428	14% 55% 30% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8190 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 REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	1	1
			4504	2914	746	835	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	HIS	-	expression tag	UNP P03366
A	559	HIS	-	expression tag	UNP P03366
A	560	HIS	-	expression tag	UNP P03366
A	561	HIS	-	expression tag	UNP P03366
A	562	HIS	-	expression tag	UNP P03366
A	57	SER	ASN	conflict	UNP P03366
A	227	CYS	PHE	engineered mutation	UNP P03366
A	478	GLN	GLU	engineered mutation	UNP P03366

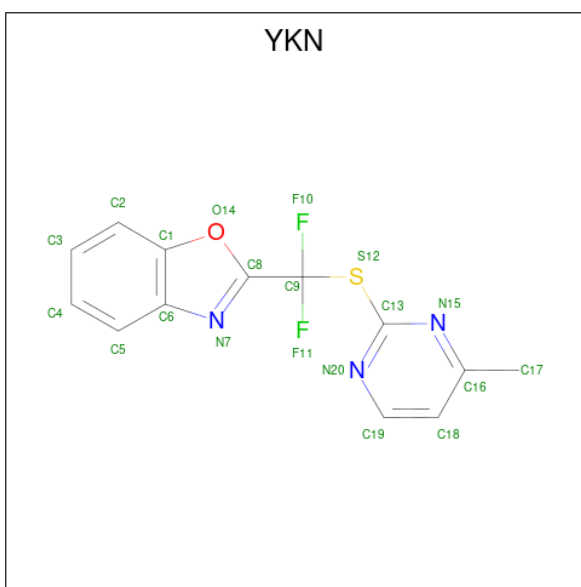
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	0	1	1
			3389	2211	557	615	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	conflict	UNP P03366

- Molecule 3 is 2-[DIFLUORO-[(4-METHYL-PYRIMIDINYL)-THIO]METHYL]-BENZOXAZOLE (CCD ID: YKN) (formula: C₁₃H₉F₂N₃OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			20	13	2	3	1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

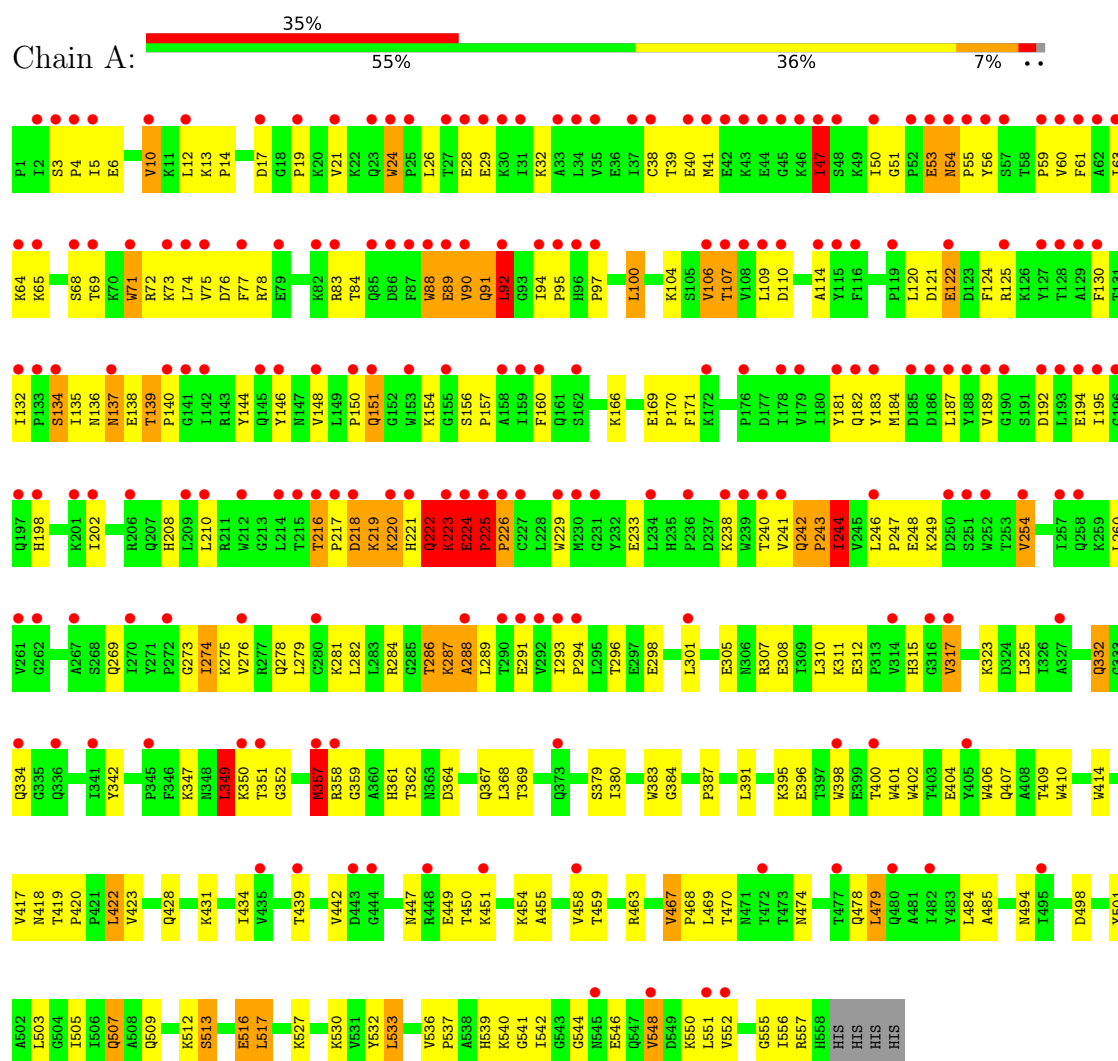
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	111	Total	O	0	0
			111	111		

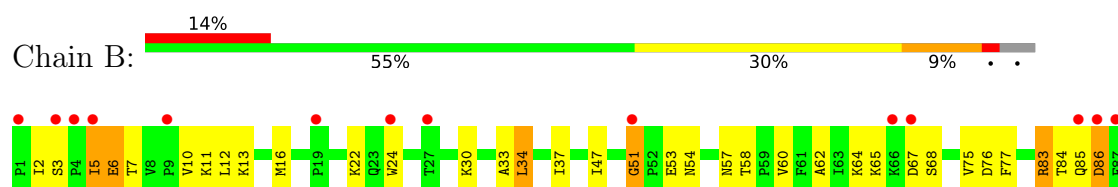
3 Residue-property plots

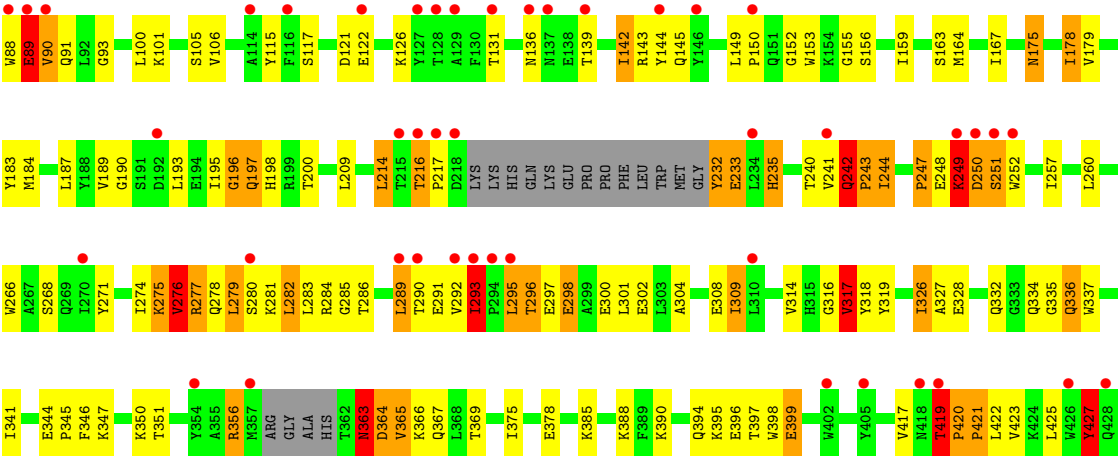
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2: REVERSE TRANSCRIPTASE/RIBONUCLEASE H





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.05Å 155.58Å 152.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.90) 99.7 (30.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.220 , 0.290 0.309 , 0.353	Depositor DCC
R_{free} test set	1813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8190	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: YKN, CA

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	0.87	3/4624 (0.1%)	1.12	16/6286 (0.3%)
2	B	0.90	1/3490 (0.0%)	1.32	25/4747 (0.5%)
All	All	0.88	4/8114 (0.0%)	1.21	41/11033 (0.4%)

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
1	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	ARG	C-N	-6.73	1.24	1.33
2	B	427	TYR	C-N	-6.73	1.24	1.33
1	A	470	THR	N-CA	5.07	1.51	1.46
1	A	225	PRO	CA-C	5.04	1.56	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	TYR	O-C-N	-27.72	78.65	123.00
2	B	427	TYR	CA-C-O	-23.26	81.26	120.80
2	B	427	TYR	CA-C-N	21.85	159.91	116.20
2	B	293	ILE	N-CA-C	13.69	124.20	108.05
1	A	225	PRO	N-CA-C	10.23	123.18	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	CA-C-N	9.79	130.46	120.38
1	A	224	GLU	C-N-CA	9.79	130.46	120.38
2	B	419	THR	CA-C-N	9.58	130.24	120.38
2	B	419	THR	C-N-CA	9.58	130.24	120.38
1	A	349	LEU	N-CA-C	-8.65	101.93	111.36
2	B	196	GLY	N-CA-C	-8.35	101.36	112.14
1	A	470	THR	N-CA-C	7.49	122.50	111.34
2	B	293	ILE	CA-C-N	6.98	128.56	119.84
2	B	293	ILE	C-N-CA	6.98	128.56	119.84
2	B	51	GLY	CA-C-N	6.75	126.38	119.56
2	B	51	GLY	C-N-CA	6.75	126.38	119.56
2	B	235	HIS	CA-C-N	6.71	126.50	119.05
2	B	235	HIS	C-N-CA	6.71	126.50	119.05
2	B	216	THR	CA-C-N	6.59	126.97	119.92
2	B	216	THR	C-N-CA	6.59	126.97	119.92
2	B	7	THR	N-CA-C	6.27	120.04	109.76
1	A	254	VAL	CB-CA-C	-6.16	103.99	111.88
2	B	131	THR	CA-C-N	-5.92	118.57	122.60
2	B	131	THR	C-N-CA	-5.92	118.57	122.60
1	A	242	GLN	CA-C-N	-5.92	112.44	119.84
1	A	242	GLN	C-N-CA	-5.92	112.44	119.84
1	A	184	MET	CB-CA-C	-5.79	109.89	116.54
1	A	368	LEU	N-CA-C	-5.71	104.67	111.69
2	B	276	VAL	N-CA-C	5.63	121.06	109.34
2	B	242	GLN	N-CA-C	5.54	122.06	109.81
2	B	249	LYS	N-CA-C	-5.51	107.13	112.97
2	B	86	ASP	N-CA-C	-5.48	105.72	112.90
2	B	84	THR	N-CA-C	-5.40	107.70	114.56
2	B	317	VAL	N-CA-C	5.38	115.65	108.11
1	A	513	SER	N-CA-C	5.32	117.17	108.76
1	A	242	GLN	N-CA-C	5.31	121.54	109.81
1	A	47	ILE	CB-CA-C	5.24	118.51	110.55
2	B	277	ARG	N-CA-C	5.22	116.78	111.14
1	A	223	LYS	N-CA-C	5.04	115.97	108.31
1	A	13	LYS	CA-C-N	5.03	126.13	119.84
1	A	13	LYS	C-N-CA	5.03	126.13	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TRP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	427	TYR	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	4504	0	4548	182	0
2	B	3389	0	3416	153	0
3	A	20	0	9	1	0
4	A	1	0	0	0	0
5	A	165	0	0	11	0
5	B	111	0	0	14	0
All	All	8190	0	7973	326	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 21.

All (326) 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:420:PRO:HB3	5:B:2111:HOH:O	1.25	1.28
1:A:107:THR:HG21	1:A:202:ILE:CD1	1.76	1.15
1:A:107:THR:HG21	1:A:202:ILE:HD11	1.22	1.12
1:A:223:LYS:HG3	1:A:224:GLU:N	1.68	1.03
1:A:223:LYS:CG	1:A:224:GLU:H	1.68	1.03
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.05	1.01
1:A:107:THR:CG2	1:A:202:ILE:HD11	1.94	0.98
1:A:54:ASN:ND2	1:A:55:PRO:O	1.96	0.97
1:A:223:LYS:HG3	1:A:224:GLU:H	0.83	0.96
2:B:281:LYS:O	2:B:282:LEU:HB2	1.62	0.96
1:A:362:THR:HG21	1:A:367:GLN:HE21	1.31	0.93
1:A:89:GLU:O	1:A:90:VAL:HG22	1.67	0.93
1:A:494:ASN:HD22	1:A:532:TYR:HB3	1.35	0.92
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.51	0.90
2:B:363:ASN:HB3	5:B:2098:HOH:O	1.71	0.90
1:A:107:THR:HA	1:A:223:LYS:HD2	1.53	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:GLY:O	2:B:197:GLN:HB3	1.73	0.88
2:B:363:ASN:O	2:B:364:ASP:HB2	1.74	0.85
2:B:337:TRP:HE1	2:B:367:GLN:NE2	1.73	0.85
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.11	0.85
1:A:361:HIS:HD2	1:A:513:SER:OG	1.59	0.84
1:A:516:GLU:OE1	1:A:516:GLU:HA	1.77	0.82
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.15	0.82
1:A:434:ILE:H	1:A:494:ASN:HD21	1.26	0.79
2:B:337:TRP:NE1	2:B:367:GLN:HE21	1.81	0.79
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.20	0.77
2:B:243:PRO:HG3	2:B:351:THR:OG1	1.85	0.77
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.67	0.77
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.66	0.76
1:A:383:TRP:O	5:A:2112:HOH:O	2.03	0.76
2:B:51:GLY:O	5:B:2019:HOH:O	2.04	0.75
1:A:233:GLU:HG3	1:A:242:GLN:HB3	1.69	0.75
2:B:326:ILE:CD1	2:B:390:LYS:HD2	2.17	0.74
1:A:89:GLU:HG2	1:A:91:GLN:H	1.50	0.74
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.69	0.74
1:A:240:THR:HG22	1:A:241:VAL:H	1.53	0.74
2:B:421:PRO:HB2	2:B:423:VAL:HG23	1.69	0.73
1:A:89:GLU:HG2	1:A:91:GLN:N	2.03	0.73
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.71	0.72
2:B:249:LYS:HB2	2:B:252:TRP:NE1	2.04	0.72
1:A:182:GLN:HB3	5:A:2075:HOH:O	1.87	0.72
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.70	0.72
1:A:61:PHE:CE2	1:A:74:LEU:HD12	2.24	0.71
1:A:121:ASP:O	1:A:122:GLU:CB	2.38	0.71
2:B:326:ILE:HD11	2:B:390:LYS:HD2	1.71	0.69
1:A:396:GLU:O	1:A:400:THR:HG22	1.92	0.69
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.10	0.69
2:B:297:GLU:HG3	2:B:298:GLU:HG3	1.75	0.68
2:B:365:VAL:O	2:B:369:THR:HG23	1.93	0.68
2:B:297:GLU:HA	2:B:300:GLU:OE2	1.93	0.68
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.74	0.68
2:B:247:PRO:HB2	2:B:250:ASP:CB	2.24	0.68
1:A:32:LYS:HD2	5:A:2009:HOH:O	1.94	0.68
2:B:12:LEU:HD23	2:B:16:MET:O	1.93	0.67
2:B:150:PRO:HD2	2:B:153:TRP:HE3	1.58	0.67
1:A:136:ASN:O	1:A:138:GLU:N	2.27	0.67
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.13	0.66
2:B:319:TYR:OH	2:B:385:LYS:HD2	1.96	0.66
1:A:136:ASN:ND2	5:A:2057:HOH:O	2.03	0.66
2:B:326:ILE:HD12	2:B:327:ALA:N	2.10	0.65
1:A:229:TRP:CD2	3:A:1559:YKN:H4	2.31	0.65
1:A:76:ASP:OD1	1:A:78:ARG:HG2	1.96	0.65
1:A:362:THR:HG21	1:A:367:GLN:NE2	2.09	0.65
2:B:363:ASN:HB3	2:B:366:LYS:HB3	1.79	0.65
1:A:220:LYS:NZ	1:A:222:GLN:OE1	2.27	0.65
1:A:498:ASP:HA	1:A:536:VAL:O	1.97	0.64
1:A:84:THR:O	1:A:154:LYS:NZ	2.28	0.64
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.79	0.64
2:B:115:TYR:OH	2:B:184:MET:O	2.16	0.64
1:A:247:PRO:O	1:A:307:ARG:NH2	2.31	0.64
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.51	0.64
1:A:97:PRO:HA	1:A:100:LEU:HD22	1.80	0.63
2:B:251:SER:O	2:B:252:TRP:CE3	2.51	0.63
2:B:5:ILE:HG13	2:B:6:GLU:N	2.11	0.63
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.80	0.63
1:A:218:ASP:HB2	1:A:222:GLN:HB2	1.79	0.63
2:B:13:LYS:HD2	2:B:86:ASP:HB2	1.79	0.63
2:B:88:TRP:C	2:B:90:VAL:H	2.05	0.63
2:B:395:LYS:O	2:B:399:GLU:HG2	1.99	0.62
1:A:494:ASN:ND2	1:A:532:TYR:HB3	2.12	0.62
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.35	0.62
2:B:11:LYS:HG3	2:B:12:LEU:O	1.99	0.62
2:B:247:PRO:HB2	2:B:250:ASP:HB2	1.80	0.62
1:A:273:GLY:O	1:A:275:LYS:HG3	2.00	0.61
1:A:361:HIS:CD2	1:A:513:SER:OG	2.50	0.61
1:A:406:TRP:CE3	2:B:420:PRO:HG3	2.35	0.61
1:A:240:THR:HG22	1:A:241:VAL:N	2.16	0.61
1:A:406:TRP:HE3	1:A:407:GLN:HE21	1.48	0.61
1:A:463:ARG:HG2	5:A:2151:HOH:O	2.00	0.61
2:B:385:LYS:HE2	5:B:2087:HOH:O	2.01	0.60
1:A:219:LYS:H	1:A:219:LYS:HD2	1.66	0.60
1:A:4:PRO:HA	5:A:2002:HOH:O	2.02	0.60
1:A:216:THR:HB	1:A:218:ASP:OD1	2.01	0.60
2:B:268:SER:HB3	2:B:274:ILE:HB	1.82	0.60
2:B:282:LEU:HG	2:B:295:LEU:HB3	1.82	0.60
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.66	0.60
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ALA:CB	1:A:469:LEU:HD11	2.31	0.60
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.85	0.59
1:A:90:VAL:O	1:A:91:GLN:HB2	2.00	0.59
2:B:314:VAL:HB	2:B:317:VAL:CG1	2.33	0.59
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.64	0.59
1:A:541:GLY:HA2	1:A:546:GLU:OE1	2.03	0.59
2:B:243:PRO:O	2:B:244:ILE:C	2.46	0.58
1:A:90:VAL:HG12	5:A:2033:HOH:O	2.03	0.58
1:A:254:VAL:HG21	1:A:288:ALA:O	2.03	0.58
2:B:214:LEU:HD12	2:B:217:PRO:HG3	1.85	0.58
1:A:417:VAL:HG13	1:A:419:THR:HG23	1.87	0.57
1:A:551:LEU:HD22	5:A:2152:HOH:O	2.04	0.57
2:B:85:GLN:NE2	2:B:88:TRP:HB2	2.20	0.57
2:B:346:PHE:HD1	5:B:2096:HOH:O	1.88	0.57
2:B:257:ILE:CD1	2:B:293:ILE:HG21	2.35	0.56
1:A:219:LYS:O	1:A:220:LYS:HG3	2.04	0.56
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.40	0.56
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.36	0.56
2:B:6:GLU:HA	5:B:2001:HOH:O	2.06	0.56
2:B:142:ILE:HD13	2:B:142:ILE:N	2.21	0.56
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.88	0.56
1:A:357:MET:O	1:A:359:GLY:N	2.33	0.56
2:B:350:LYS:CE	2:B:378:GLU:OE1	2.54	0.56
2:B:279:LEU:O	2:B:281:LYS:O	2.24	0.56
2:B:196:GLY:O	2:B:197:GLN:CB	2.43	0.55
1:A:63:ILE:HG13	1:A:64:LYS:H	1.71	0.55
2:B:88:TRP:C	2:B:90:VAL:N	2.64	0.55
2:B:417:VAL:HG12	2:B:419:THR:O	2.06	0.55
1:A:134:SER:HB2	1:A:139:THR:O	2.05	0.55
1:A:218:ASP:CB	1:A:222:GLN:HB2	2.35	0.55
2:B:150:PRO:HD2	2:B:153:TRP:CE3	2.41	0.55
2:B:283:LEU:O	2:B:285:GLY:N	2.39	0.55
1:A:106:VAL:HA	1:A:189:VAL:O	2.07	0.55
1:A:450:THR:O	1:A:451:LYS:HB2	2.07	0.55
2:B:241:VAL:HG13	2:B:242:GLN:H	1.72	0.55
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.88	0.54
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.55	0.54
2:B:252:TRP:O	2:B:293:ILE:HG13	2.07	0.54
2:B:326:ILE:HD13	2:B:390:LYS:HD2	1.88	0.54
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.08	0.54
2:B:420:PRO:HD2	2:B:420:PRO:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.90	0.54
2:B:77:PHE:HD2	2:B:152:GLY:HA3	1.71	0.54
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.43	0.53
2:B:286:THR:HG22	2:B:286:THR:O	2.07	0.53
2:B:257:ILE:HD11	2:B:293:ILE:HG21	1.90	0.53
2:B:197:GLN:HB2	5:B:2064:HOH:O	2.08	0.53
1:A:121:ASP:O	1:A:122:GLU:HB2	2.09	0.53
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.43	0.53
1:A:64:LYS:HD2	1:A:69:THR:HA	1.91	0.53
1:A:120:LEU:HD12	1:A:121:ASP:H	1.74	0.53
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.90	0.53
2:B:88:TRP:N	2:B:88:TRP:CD1	2.75	0.53
1:A:122:GLU:CA	1:A:125:ARG:HG3	2.38	0.52
1:A:240:THR:OG1	1:A:315:HIS:ND1	2.43	0.52
2:B:275:LYS:HB2	2:B:302:GLU:HG3	1.89	0.52
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.50	0.52
1:A:60:VAL:CG1	1:A:130:PHE:CD2	2.91	0.52
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.92	0.52
2:B:292:VAL:HG22	2:B:293:ILE:H	1.75	0.52
1:A:88:TRP:CD2	1:A:89:GLU:HB2	2.45	0.52
1:A:401:TRP:CD1	1:A:402:TRP:CD1	2.96	0.51
1:A:402:TRP:CD2	1:A:409:THR:HG21	2.46	0.51
1:A:223:LYS:O	1:A:224:GLU:HB2	2.10	0.51
2:B:249:LYS:HB2	2:B:252:TRP:HE1	1.72	0.51
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.91	0.51
2:B:83:ARG:NH2	5:B:2033:HOH:O	2.42	0.51
2:B:164:MET:HE1	2:B:209:LEU:HD21	1.92	0.51
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.98	0.51
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.51
1:A:89:GLU:HG2	1:A:91:GLN:CA	2.39	0.51
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.93	0.51
2:B:278:GLN:O	2:B:282:LEU:HD12	2.10	0.51
2:B:420:PRO:O	2:B:420:PRO:CD	2.58	0.51
2:B:281:LYS:O	2:B:282:LEU:CB	2.42	0.51
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.46	0.51
1:A:281:LYS:HE2	1:A:284:ARG:NH2	2.26	0.50
1:A:47:ILE:HG23	1:A:144:TYR:CD1	2.46	0.50
2:B:106:VAL:HA	2:B:189:VAL:O	2.11	0.50
2:B:356:ARG:HG2	2:B:356:ARG:NH1	2.26	0.50
1:A:121:ASP:O	1:A:122:GLU:HB3	2.10	0.50
1:A:395:LYS:HD2	1:A:414:TRP:CZ3	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:TYR:HA	5:B:2086:HOH:O	2.12	0.50
1:A:287:LYS:O	1:A:288:ALA:HB3	2.11	0.50
1:A:89:GLU:HG2	1:A:91:GLN:HA	1.92	0.50
2:B:232:TYR:HD1	2:B:233:GLU:H	1.59	0.49
2:B:89:GLU:HA	2:B:93:GLY:HA2	1.93	0.49
1:A:89:GLU:C	1:A:91:GLN:H	2.19	0.49
2:B:64:LYS:HD3	2:B:68:SER:H	1.76	0.49
1:A:169:GLU:N	1:A:170:PRO:HD2	2.28	0.49
2:B:77:PHE:HD2	2:B:152:GLY:CA	2.25	0.49
2:B:350:LYS:HE3	2:B:378:GLU:OE1	2.12	0.49
2:B:175:ASN:HB3	2:B:178:ILE:HD13	1.94	0.49
2:B:295:LEU:O	2:B:296:THR:OG1	2.26	0.49
1:A:223:LYS:CG	1:A:224:GLU:N	2.44	0.48
2:B:54:ASN:O	2:B:143:ARG:NH2	2.46	0.48
2:B:195:ILE:O	2:B:198:HIS:HB3	2.12	0.48
2:B:266:TRP:HH2	2:B:427:TYR:HH	1.60	0.48
2:B:247:PRO:HB2	2:B:250:ASP:HB3	1.95	0.48
2:B:327:ALA:HB2	2:B:341:ILE:HD13	1.95	0.48
1:A:90:VAL:CG1	5:A:2033:HOH:O	2.60	0.48
2:B:232:TYR:O	2:B:233:GLU:CB	2.62	0.48
2:B:248:GLU:C	2:B:250:ASP:H	2.20	0.48
1:A:39:THR:O	1:A:40:GLU:C	2.57	0.48
1:A:317:VAL:HG23	1:A:349:LEU:HD22	1.96	0.48
1:A:51:GLY:HA3	1:A:53:GLU:HG2	1.96	0.47
2:B:89:GLU:HA	2:B:93:GLY:CA	2.44	0.47
2:B:271:TYR:HB3	2:B:309:ILE:HD11	1.95	0.47
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.49	0.47
1:A:166:LYS:NZ	5:A:2065:HOH:O	2.45	0.47
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.13	0.47
1:A:474:ASN:O	1:A:478:GLN:HG2	2.14	0.47
1:A:479:LEU:CB	1:A:517:LEU:HD13	2.43	0.47
2:B:121:ASP:OD1	2:B:121:ASP:C	2.58	0.47
1:A:216:THR:O	1:A:218:ASP:N	2.48	0.47
2:B:334:GLN:O	2:B:334:GLN:HG3	2.15	0.47
1:A:28:GLU:O	1:A:29:GLU:C	2.57	0.47
1:A:136:ASN:O	1:A:137:ASN:C	2.58	0.47
1:A:243:PRO:CG	1:A:244:ILE:N	2.74	0.47
2:B:33:ALA:O	2:B:37:ILE:HD12	2.15	0.47
1:A:418:ASN:O	1:A:420:PRO:HD3	2.15	0.47
2:B:367:GLN:NE2	5:B:2092:HOH:O	2.48	0.47
1:A:410:TRP:HB2	2:B:365:VAL:HG13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:GLY:HA3	5:B:2085:HOH:O	2.15	0.47
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.96	0.47
1:A:88:TRP:CZ2	2:B:143:ARG:HD2	2.49	0.46
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.14	0.46
1:A:19:PRO:O	1:A:56:TYR:HA	2.16	0.46
2:B:11:LYS:HE3	2:B:12:LEU:O	2.14	0.46
2:B:394:GLN:HB3	2:B:397:THR:OG1	2.15	0.46
1:A:24:TRP:H	1:A:24:TRP:CD1	2.30	0.46
2:B:100:LEU:HD13	2:B:179:VAL:HG12	1.97	0.46
1:A:406:TRP:CE3	1:A:407:GLN:HG2	2.51	0.46
1:A:351:THR:HG22	1:A:352:GLY:N	2.30	0.46
2:B:11:LYS:HA	2:B:11:LYS:HD2	1.85	0.46
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.97	0.46
2:B:260:LEU:HD13	2:B:260:LEU:O	2.15	0.46
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.98	0.46
2:B:318:TYR:HD2	5:B:2086:HOH:O	1.99	0.46
2:B:214:LEU:HD12	2:B:217:PRO:CG	2.44	0.46
2:B:335:GLY:HA2	2:B:367:GLN:HE22	1.80	0.46
2:B:304:ALA:O	2:B:308:GLU:HG2	2.16	0.46
2:B:332:GLN:HB2	2:B:336:GLN:HB2	1.97	0.45
1:A:77:PHE:O	1:A:78:ARG:C	2.59	0.45
5:A:2141:HOH:O	2:B:290:THR:OG1	2.21	0.45
2:B:58:THR:HG23	2:B:76:ASP:O	2.15	0.45
1:A:362:THR:CG2	1:A:367:GLN:HE21	2.14	0.45
2:B:297:GLU:HG3	2:B:298:GLU:H	1.81	0.45
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.46	0.45
1:A:439:THR:HG23	2:B:289:LEU:HD22	1.98	0.45
1:A:507:GLN:O	1:A:509[B]:GLN:NE2	2.50	0.44
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.52	0.44
1:A:3:SER:HB3	1:A:5:ILE:HG22	1.98	0.44
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.83	0.44
2:B:53:GLU:OE1	2:B:53:GLU:N	2.43	0.44
2:B:297:GLU:CG	2:B:298:GLU:H	2.30	0.44
1:A:107:THR:HG22	1:A:198:HIS:NE2	2.33	0.44
2:B:363:ASN:O	2:B:364:ASP:CB	2.54	0.44
1:A:28:GLU:HG2	1:A:135:ILE:HG12	2.00	0.43
1:A:293:ILE:HA	1:A:294:PRO:HD2	1.81	0.43
1:A:146:TYR:OH	1:A:151:GLN:NE2	2.51	0.43
1:A:308:GLU:OE1	1:A:308:GLU:HA	2.17	0.43
1:A:447:ASN:C	1:A:449:GLU:H	2.26	0.43
2:B:155:GLY:O	2:B:159:ILE:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:MET:HE2	2:B:187:LEU:HD11	2.00	0.43
2:B:390:LYS:HB3	2:B:417:VAL:CG2	2.48	0.43
1:A:362:THR:CG2	1:A:367:GLN:NE2	2.79	0.43
1:A:458:VAL:HG23	1:A:548:VAL:HG13	2.00	0.43
1:A:216:THR:C	1:A:218:ASP:H	2.26	0.43
1:A:269:GLN:C	1:A:351:THR:HB	2.44	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.49	0.43
1:A:61:PHE:HE2	1:A:74:LEU:HD12	1.82	0.43
1:A:224:GLU:HA	1:A:225:PRO:HD2	1.74	0.43
1:A:273:GLY:O	1:A:274:ILE:C	2.62	0.43
1:A:41:MET:HE1	1:A:73:LYS:HE3	2.01	0.43
1:A:95:PRO:HB3	2:B:136:ASN:ND2	2.34	0.43
1:A:281:LYS:HE2	1:A:284:ARG:HH22	1.84	0.43
1:A:537:PRO:HD2	1:A:542:ILE:HD13	2.01	0.42
1:A:24:TRP:HH2	1:A:61:PHE:CD1	2.37	0.42
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.54	0.42
2:B:328:GLU:CG	2:B:390:LYS:HD3	2.49	0.42
2:B:366:LYS:HB3	5:B:2098:HOH:O	2.18	0.42
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.83	0.42
2:B:149:LEU:HB3	2:B:156:SER:OG	2.19	0.42
2:B:183:TYR:HA	5:B:2059:HOH:O	2.20	0.42
2:B:247:PRO:HG2	2:B:250:ASP:HB2	2.01	0.42
2:B:251:SER:O	2:B:252:TRP:HE3	2.00	0.42
1:A:88:TRP:CG	1:A:89:GLU:HB2	2.54	0.42
2:B:214:LEU:HD22	2:B:214:LEU:HA	1.84	0.42
1:A:89:GLU:HA	1:A:92:LEU:HD13	2.01	0.42
1:A:156:SER:N	1:A:157:PRO:CD	2.83	0.42
1:A:17:ASP:O	1:A:83:ARG:HD3	2.19	0.42
2:B:292:VAL:HG22	2:B:293:ILE:N	2.34	0.42
1:A:194:GLU:O	1:A:195:ILE:C	2.63	0.42
2:B:241:VAL:HG22	2:B:243:PRO:HD3	2.01	0.42
2:B:30:LYS:O	2:B:34:LEU:HB2	2.21	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.41
1:A:10:VAL:HG22	1:A:124:PHE:CD1	2.55	0.41
1:A:216:THR:C	1:A:218:ASP:N	2.78	0.41
1:A:6:GLU:CD	1:A:6:GLU:H	2.28	0.41
1:A:53:GLU:HG2	1:A:53:GLU:H	1.59	0.41
1:A:55:PRO:O	1:A:56:TYR:HB2	2.20	0.41
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.55	0.41
1:A:391:LEU:HD12	1:A:414:TRP:CD2	2.55	0.41
1:A:454:LYS:HD2	1:A:555:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:HD12	2:B:144:TYR:CG	2.56	0.41
1:A:89:GLU:HB3	1:A:90:VAL:H	1.73	0.41
1:A:349:LEU:N	1:A:349:LEU:CD2	2.84	0.41
1:A:548:VAL:O	1:A:552:VAL:HG23	2.21	0.41
2:B:394:GLN:HG2	2:B:396:GLU:OE1	2.20	0.41
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.51	0.40
2:B:197:GLN:HA	2:B:200:THR:HB	2.02	0.40
1:A:406:TRP:CE3	2:B:420:PRO:CG	3.04	0.40
1:A:422:LEU:H	1:A:422:LEU:HD22	1.85	0.40
1:A:467:VAL:HA	1:A:468:PRO:HD2	1.97	0.40
1:A:55:PRO:O	1:A:56:TYR:CB	2.69	0.40
1:A:54:ASN:HD21	1:A:56:TYR:HD2	1.68	0.40
1:A:148:VAL:O	1:A:150:PRO:HD3	2.22	0.40
1:A:219:LYS:C	1:A:220:LYS:HG3	2.47	0.40
1:A:275:LYS:HD2	1:A:332:GLN:NE2	2.37	0.40
1:A:282:LEU:CD2	1:A:296:THR:HG23	2.51	0.40
2:B:105:SER:OG	2:B:235:HIS:CD2	2.75	0.40
1:A:380:ILE:O	1:A:384:GLY:HA2	2.21	0.40
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.57	0.40
1:A:544:GLY:N	2:B:285:GLY:O	2.55	0.40
2:B:34:LEU:HD13	2:B:62:ALA:HB2	2.02	0.40
2:B:90:VAL:HG22	2:B:91:GLN:N	2.36	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	557/562 (99%)	489 (88%)	45 (8%)	23 (4%)	2	9
2	B	406/428 (95%)	352 (87%)	39 (10%)	15 (4%)	2	11
All	All	963/990 (97%)	841 (87%)	84 (9%)	38 (4%)	2	10

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	122	GLU
1	A	137	ASN
1	A	224	GLU
1	A	243	PRO
2	B	2	ILE
2	B	243	PRO
2	B	244	ILE
2	B	276	VAL
2	B	284	ARG
2	B	363	ASN
2	B	420	PRO
1	A	90	VAL
1	A	222	GLN
1	A	225	PRO
1	A	244	ILE
1	A	357	MET
1	A	358	ARG
1	A	539	HIS
2	B	197	GLN
2	B	233	GLU
2	B	296	THR
2	B	364	ASP
2	B	421	PRO
1	A	226	PRO
2	B	89	GLU
1	A	286	THR
1	A	334	GLN
2	B	242	GLN
2	B	247	PRO
1	A	71	TRP
1	A	89	GLU
1	A	92	LEU
1	A	217	PRO
1	A	288	ALA
1	A	14	PRO
1	A	556	ILE
1	A	274	ILE

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	493/502 (98%)	423 (86%)	70 (14%)	3	11
2	B	373/390 (96%)	321 (86%)	52 (14%)	3	11
All	All	866/892 (97%)	744 (86%)	122 (14%)	3	11

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	12	LEU
1	A	24	TRP
1	A	26	LEU
1	A	47	ILE
1	A	50	ILE
1	A	53	GLU
1	A	54	ASN
1	A	65	LYS
1	A	68	SER
1	A	71	TRP
1	A	72	ARG
1	A	92	LEU
1	A	94	ILE
1	A	100	LEU
1	A	106	VAL
1	A	107	THR
1	A	110	ASP
1	A	134	SER
1	A	139	THR
1	A	151	GLN
1	A	187	LEU
1	A	210	LEU
1	A	216	THR
1	A	218	ASP
1	A	219	LYS
1	A	220	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	221	HIS
1	A	222	GLN
1	A	223	LYS
1	A	238	LYS
1	A	244	ILE
1	A	248	GLU
1	A	249	LYS
1	A	260	LEU
1	A	276	VAL
1	A	279	LEU
1	A	286	THR
1	A	287	LYS
1	A	289	LEU
1	A	291	GLU
1	A	301	LEU
1	A	305	GLU
1	A	311	LYS
1	A	312	GLU
1	A	317	VAL
1	A	323	LYS
1	A	325	LEU
1	A	332	GLN
1	A	347	LYS
1	A	349	LEU
1	A	357	MET
1	A	404	GLU
1	A	422	LEU
1	A	428	GLN
1	A	431	LYS
1	A	459	THR
1	A	467	VAL
1	A	479	LEU
1	A	484	LEU
1	A	507	GLN
1	A	512	LYS
1	A	516	GLU
1	A	517	LEU
1	A	527	LYS
1	A	530	LYS
1	A	533	LEU
1	A	540	LYS
1	A	548	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	550	LYS
2	B	3	SER
2	B	5	ILE
2	B	6	GLU
2	B	22	LYS
2	B	34	LEU
2	B	65	LYS
2	B	67	ASP
2	B	83	ARG
2	B	89	GLU
2	B	90	VAL
2	B	101	LYS
2	B	117	SER
2	B	122	GLU
2	B	139	THR
2	B	142	ILE
2	B	175	ASN
2	B	178	ILE
2	B	193	LEU
2	B	214	LEU
2	B	216	THR
2	B	232	TYR
2	B	240	THR
2	B	249	LYS
2	B	250	ASP
2	B	251	SER
2	B	275	LYS
2	B	276	VAL
2	B	277	ARG
2	B	279	LEU
2	B	280	SER
2	B	282	LEU
2	B	289	LEU
2	B	291	GLU
2	B	293	ILE
2	B	295	LEU
2	B	298	GLU
2	B	301	LEU
2	B	309	ILE
2	B	317	VAL
2	B	326	ILE
2	B	336	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	344	GLU
2	B	345	PRO
2	B	347	LYS
2	B	356	ARG
2	B	363	ASN
2	B	365	VAL
2	B	388	LYS
2	B	399	GLU
2	B	419	THR
2	B	422	LEU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	ASN
1	A	137	ASN
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	361	HIS
1	A	367	GLN
1	A	407	GLN
1	A	464	GLN
1	A	474	ASN
1	A	494	ASN
1	A	520	GLN
1	A	539	HIS
2	B	57	ASN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	235	HIS
2	B	242	GLN
2	B	278	GLN
2	B	336	GLN
2	B	363	ASN
2	B	367	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	YKN	A	1559	-	19,22,22	2.03	3 (15%)	25,32,32	3.20	12 (48%)

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	YKN	A	1559	-	-	0/6/11/11	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1559	YKN	C13-S12	-6.08	1.67	1.76
3	A	1559	YKN	O14-C1	-4.09	1.32	1.38
3	A	1559	YKN	C8-N7	3.90	1.35	1.29

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1559	YKN	O14-C8-C9	8.36	124.53	116.85
3	A	1559	YKN	O14-C1-C6	7.16	112.66	107.80
3	A	1559	YKN	C9-C8-N7	-6.33	121.27	127.22
3	A	1559	YKN	C13-N15-C16	4.27	120.63	115.96
3	A	1559	YKN	N20-C13-N15	-4.02	122.58	127.57
3	A	1559	YKN	C1-C6-N7	-3.05	105.77	108.60
3	A	1559	YKN	C18-C19-N20	-3.04	120.25	123.97
3	A	1559	YKN	C19-N20-C13	2.75	119.02	114.96
3	A	1559	YKN	O14-C8-N7	-2.63	114.12	115.82
3	A	1559	YKN	F11-C9-F10	-2.33	102.96	106.86
3	A	1559	YKN	C5-C6-N7	2.15	134.32	128.21
3	A	1559	YKN	C4-C3-C2	2.01	122.72	120.24

There are no chirality outliers.

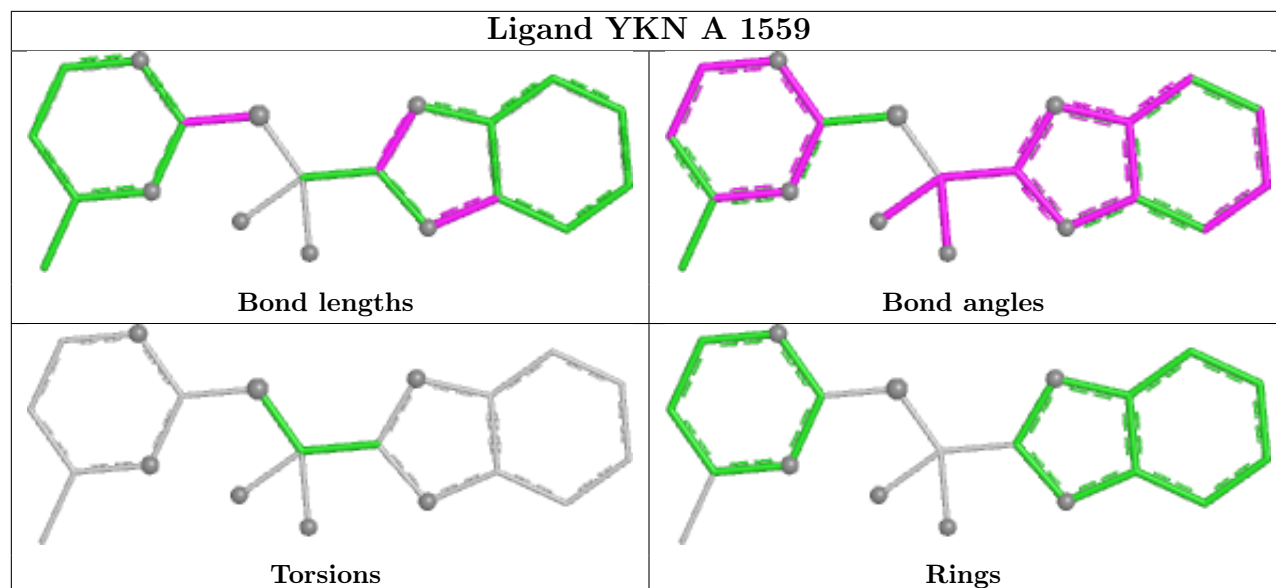
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1559	YKN	1	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	558/562 (99%)	1.70	199 (35%) 1 0	29, 53, 86, 98	1 (0%)
2	B	411/428 (96%)	1.07	58 (14%) 6 5	25, 53, 92, 106	1 (0%)
All	All	969/990 (97%)	1.44	257 (26%) 1 1	25, 53, 90, 106	2 (0%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	ILE	5.9
2	B	86	ASP	5.6
1	A	38	CYS	5.6
1	A	317	VAL	5.5
1	A	150	PRO	5.3
2	B	250	ASP	5.2
2	B	294	PRO	5.2
2	B	3	SER	4.7
1	A	221	HIS	4.7
1	A	63	ILE	4.5
1	A	50	ILE	4.4
1	A	140	PRO	4.4
1	A	62	ALA	4.3
1	A	24	TRP	4.3
1	A	47	ILE	4.2
1	A	69	THR	4.1
1	A	27	THR	4.0
2	B	217	PRO	4.0
1	A	34	LEU	4.0
1	A	60	VAL	4.0
1	A	215	THR	3.9
1	A	162	SER	3.9
1	A	3	SER	3.7
1	A	314	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	216	THR	3.6
1	A	316	GLY	3.6
1	A	254	VAL	3.6
1	A	551	LEU	3.6
1	A	146	TYR	3.5
2	B	293	ILE	3.5
1	A	197	GLN	3.5
1	A	252	TRP	3.5
1	A	77	PHE	3.4
1	A	109	LEU	3.4
1	A	90	VAL	3.4
1	A	195	ILE	3.4
1	A	141	GLY	3.3
1	A	220	LYS	3.3
1	A	134	SER	3.3
1	A	218	ASP	3.3
1	A	155	GLY	3.3
2	B	418	ASN	3.3
1	A	35	VAL	3.3
1	A	128	THR	3.3
1	A	133	PRO	3.2
1	A	272	PRO	3.2
1	A	230	MET	3.2
1	A	145	GLN	3.2
1	A	183	TYR	3.2
1	A	96	HIS	3.2
1	A	21	VAL	3.2
2	B	85	GLN	3.2
2	B	127	TYR	3.2
1	A	448	ARG	3.2
1	A	159	ILE	3.2
1	A	41	MET	3.2
2	B	88	TRP	3.2
1	A	87	PHE	3.1
2	B	295	LEU	3.1
1	A	2	ILE	3.1
1	A	55	PRO	3.1
1	A	188	TYR	3.1
1	A	186	ASP	3.1
1	A	65	LYS	3.1
1	A	88	TRP	3.1
1	A	288	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	428	GLN	3.0
1	A	241	VAL	3.0
2	B	426	TRP	3.0
1	A	54	ASN	3.0
1	A	30	LYS	3.0
1	A	194	GLU	3.0
2	B	128	THR	3.0
1	A	158	ALA	3.0
2	B	357	MET	3.0
1	A	132	ILE	3.0
1	A	223	LYS	3.0
2	B	241	VAL	3.0
2	B	251	SER	3.0
1	A	209	LEU	2.9
2	B	4	PRO	2.9
1	A	64	LYS	2.9
1	A	53	GLU	2.9
1	A	48	SER	2.9
1	A	110	ASP	2.9
1	A	179	VAL	2.9
1	A	190	GLY	2.9
2	B	146	TYR	2.9
1	A	17	ASP	2.9
1	A	129	ALA	2.9
1	A	130	PHE	2.9
1	A	227	CYS	2.9
1	A	231	GLY	2.8
2	B	136	ASN	2.8
1	A	37	ILE	2.8
1	A	472	THR	2.8
2	B	354	TYR	2.8
1	A	189	VAL	2.8
1	A	240	THR	2.8
1	A	151	GLN	2.8
1	A	291	GLU	2.8
1	A	196	GLY	2.8
2	B	9	PRO	2.8
1	A	280	CYS	2.8
1	A	552	VAL	2.8
1	A	12	LEU	2.8
1	A	193	LEU	2.8
1	A	482	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	2.8
1	A	301	LEU	2.7
1	A	198	HIS	2.7
1	A	357	MET	2.7
1	A	106	VAL	2.7
1	A	341	ILE	2.7
1	A	351	THR	2.7
1	A	153	TRP	2.7
1	A	71	TRP	2.6
1	A	45	GLY	2.6
1	A	548	VAL	2.6
1	A	94	ILE	2.6
2	B	114	ALA	2.6
2	B	51	GLY	2.6
2	B	27	THR	2.6
2	B	218	ASP	2.6
1	A	214	LEU	2.6
1	A	42	GLU	2.6
1	A	142	ILE	2.6
1	A	258	GLN	2.6
2	B	1	PRO	2.6
2	B	19	PRO	2.6
1	A	210	LEU	2.6
1	A	148	VAL	2.6
1	A	202	ILE	2.6
1	A	290	THR	2.6
1	A	327	ALA	2.6
1	A	95	PRO	2.5
1	A	226	PRO	2.5
1	A	127	TYR	2.5
1	A	75	VAL	2.5
1	A	293	ILE	2.5
1	A	182	GLN	2.5
1	A	334	GLN	2.5
1	A	92	LEU	2.5
1	A	234	LEU	2.5
1	A	439	THR	2.5
2	B	89	GLU	2.5
1	A	246	LEU	2.5
1	A	294	PRO	2.5
1	A	89	GLU	2.5
2	B	131	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	435	VAL	2.5
2	B	24[A]	TRP	2.5
1	A	115	TYR	2.5
2	B	129	ALA	2.5
1	A	73	LYS	2.5
1	A	86	ASP	2.4
1	A	225	PRO	2.4
1	A	276	VAL	2.4
1	A	85	GLN	2.4
1	A	405	TYR	2.4
1	A	97	PRO	2.4
2	B	90	VAL	2.4
1	A	57	SER	2.4
1	A	350	LYS	2.4
1	A	239	TRP	2.4
1	A	400	THR	2.4
2	B	289	LEU	2.4
1	A	137	ASN	2.4
1	A	52	PRO	2.4
1	A	59	PRO	2.4
1	A	122	GLU	2.4
1	A	33	ALA	2.4
2	B	419	THR	2.4
1	A	358	ARG	2.4
2	B	280	SER	2.4
2	B	215	THR	2.4
1	A	46	LYS	2.3
1	A	262	GLY	2.3
1	A	79	GLU	2.3
1	A	212	TRP	2.3
2	B	252	TRP	2.3
2	B	234	LEU	2.3
2	B	310	LEU	2.3
1	A	270	ILE	2.3
2	B	144	TYR	2.3
2	B	249	LYS	2.3
1	A	19	PRO	2.3
1	A	192	ASP	2.3
1	A	172	LYS	2.3
2	B	66	LYS	2.3
2	B	270	ILE	2.3
1	A	56	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	217	PRO	2.3
1	A	250	ASP	2.3
1	A	238	LYS	2.3
1	A	229	TRP	2.3
2	B	139	THR	2.3
2	B	402	TRP	2.3
1	A	116	PHE	2.2
1	A	160	PHE	2.2
2	B	5	ILE	2.2
1	A	125	ARG	2.2
1	A	44	GLU	2.2
1	A	292	VAL	2.2
1	A	458	VAL	2.2
2	B	405	TYR	2.2
1	A	43	LYS	2.2
1	A	29	GLU	2.2
1	A	545	ASN	2.2
1	A	443	ASP	2.2
1	A	25	PRO	2.2
1	A	477	THR	2.2
1	A	68	SER	2.2
1	A	61	PHE	2.2
2	B	87	PHE	2.2
1	A	187	LEU	2.2
1	A	257	ILE	2.2
1	A	119	PRO	2.2
1	A	107	THR	2.2
1	A	336	GLN	2.1
1	A	4	PRO	2.1
1	A	236	PRO	2.1
2	B	192	ASP	2.1
1	A	82	LYS	2.1
1	A	74	LEU	2.1
1	A	181	TYR	2.1
1	A	5	ILE	2.1
1	A	108	VAL	2.1
1	A	345	PRO	2.1
1	A	451	LYS	2.1
1	A	185	ASP	2.1
1	A	206	ARG	2.1
1	A	114	ALA	2.1
1	A	267	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	28	GLU	2.1
1	A	495	ILE	2.1
1	A	10	VAL	2.1
1	A	201	LYS	2.1
2	B	292	VAL	2.1
1	A	176	PRO	2.1
2	B	150	PRO	2.1
2	B	137	ASN	2.1
1	A	444	GLY	2.1
1	A	216	THR	2.1
1	A	40	GLU	2.1
1	A	224	GLU	2.1
2	B	122	GLU	2.1
1	A	373	GLN	2.0
1	A	261	VAL	2.0
1	A	83	ARG	2.0
2	B	116	PHE	2.0
2	B	290	THR	2.0
1	A	23	GLN	2.0
1	A	251	SER	2.0
1	A	480	GLN	2.0
1	A	178	ILE	2.0
1	A	398	TRP	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](#)

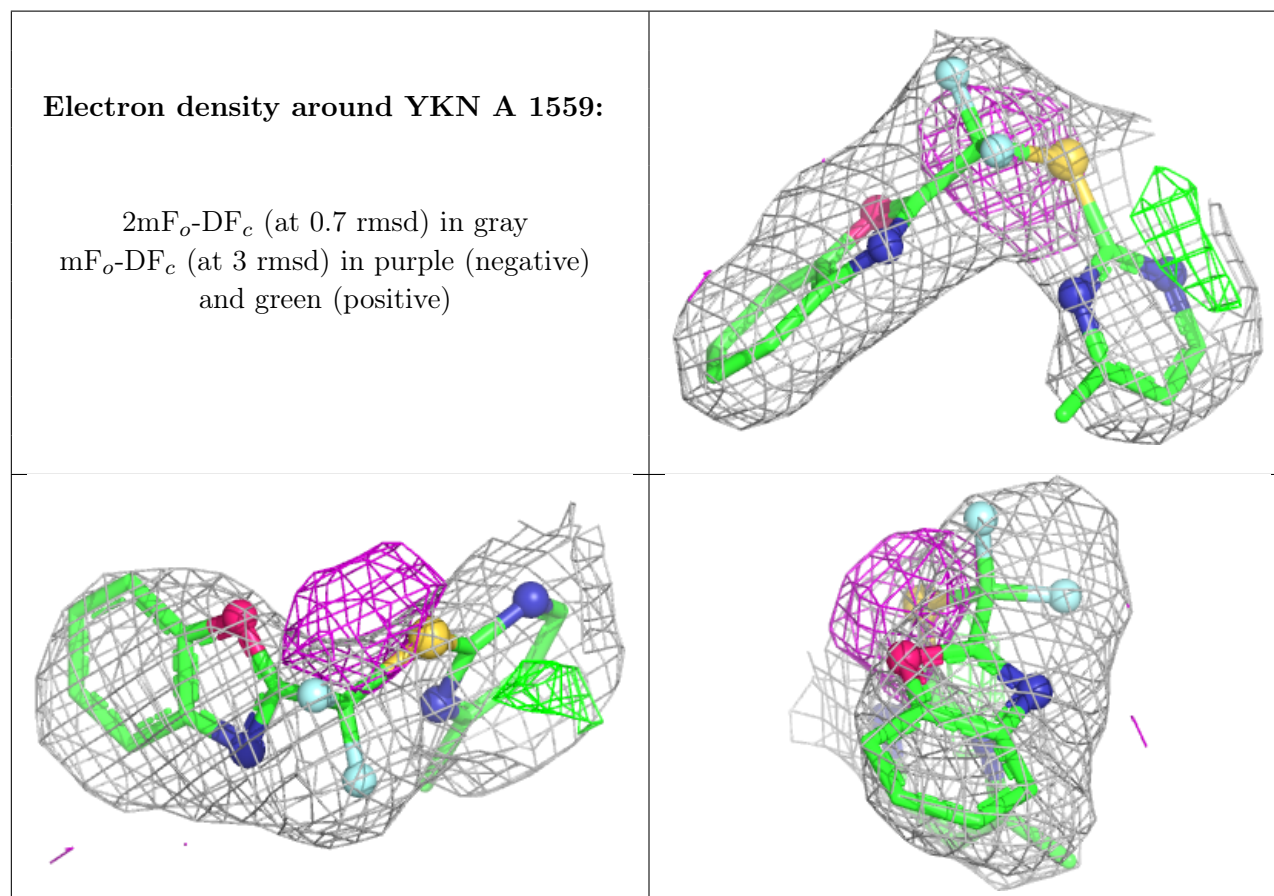
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YKN	A	1559	20/20	0.77	0.20	37,49,51,52	0
4	CA	A	1560	1/1	0.94	0.07	81,81,81,81	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 [i](#)

There are no such residues in this entry.