Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:57 am BST

PDB ID	:	2YKM
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 following versions of software and data (see references ⓘ) were used in the production of this report:

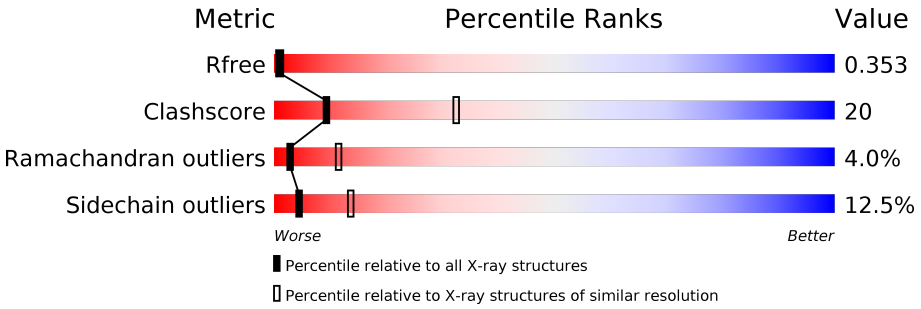
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	562	58% 34% 7% ••
2	B	428	56% 31% 8% •

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

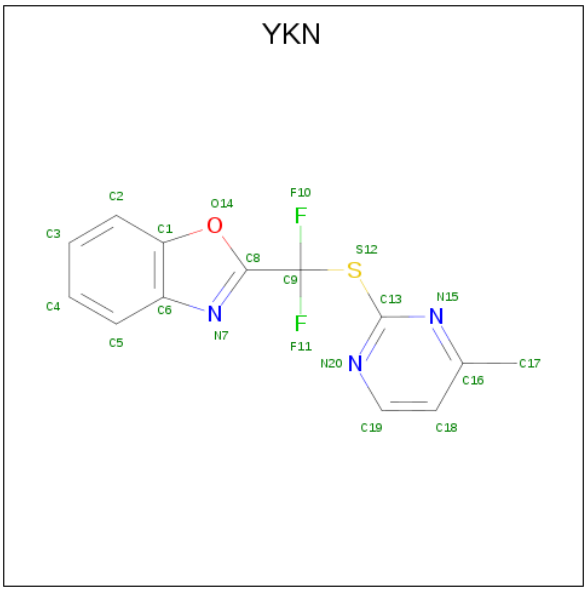
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

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 (three-letter code: YKN) (formula: $C_{13}H_9F_2N_3OS$).



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 (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

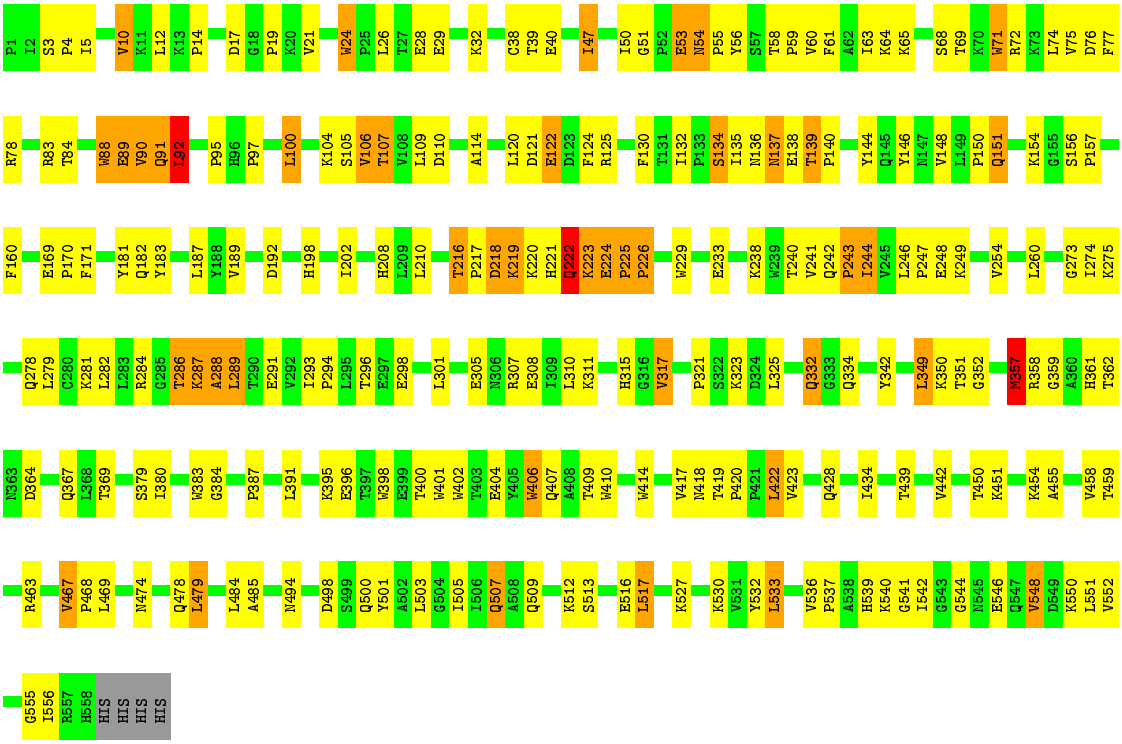
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	111	Total	O	0	0
			111	111		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

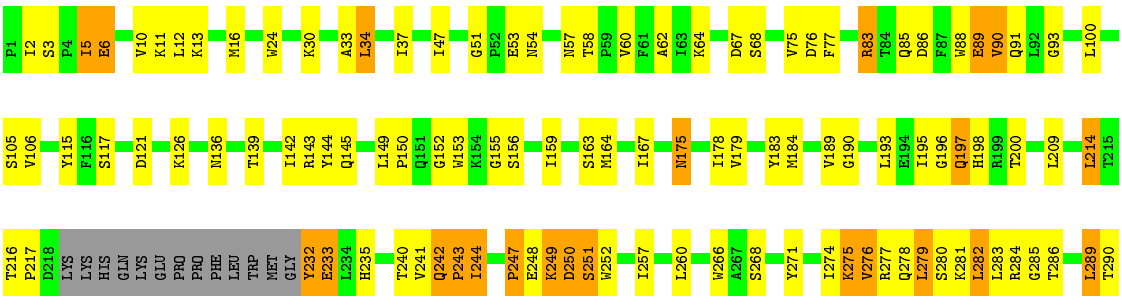
- Molecule 1: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

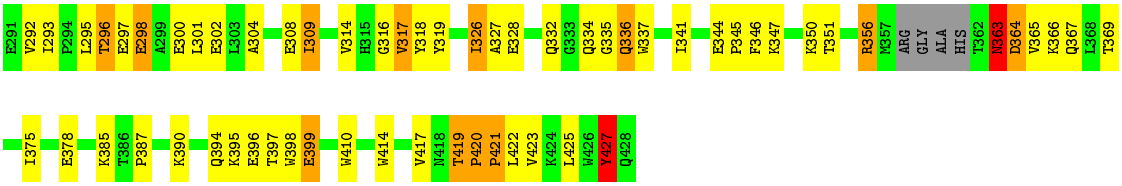
Chain A:



- Molecule 2: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

Chain B:




E291
V292
I293
P294
L295
T296
E297
E298
A299
E300
L301
E302
L303
A304
E308
I309
V314
H315
G316
V317
Y318
Y319
I326
A327
E328
Q332
G333
Q334
G335
Q336
W337
I341
E344
P345
F346
K347
K350
T351
R356
M357
ARG
GLY
ALA
HIS
T362
N363
D364
V365
K366
Q367
L368
T369
I375
E378
K385
T386
P387
K390
Q394
K395
E396
T397
W398
E399
W410
W414
V417
N418
T419
P420
P421
L422
V423
K424
L425
W426
Y427
Q428

4 Data and refinement statistics (i)

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 20.82 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.90) 98.2 (20.82-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, YKN

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	0.72	0/4624	0.79	3/6286 (0.0%)
2	B	0.72	0/3490	0.97	3/4747 (0.1%)
All	All	0.72	0/8114	0.87	6/11033 (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
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	427	TYR	O-C-N	-27.53	78.65	122.70
2	B	427	TYR	CA-C-N	19.41	159.91	117.20
2	B	427	TYR	CA-C-O	-18.50	81.26	120.10
1	A	289	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	325	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	58	THR	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TRP	Peptide
2	B	427	TYR	Mainchain

5.2 Too-close contacts (i)

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	172	0
2	B	3389	0	3416	152	0
3	A	20	0	9	1	0
4	A	1	0	0	0	0
5	A	165	0	0	10	0
5	B	111	0	0	14	0
All	All	8190	0	7973	315	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 20.

All (315) 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:HA	1:A:516:GLU:OE1	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
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
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:5:ILE:HG13	2:B:6:GLU:N	2.11	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: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
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: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:HD2	1:A:219:LYS:H	1.66	0.60
1:A:216:THR:HB	1:A:218:ASP:OD1	2.01	0.60
1:A:4:PRO:HA	5:A:2002:HOH:O	2.02	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
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.51	0.60
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.66	0.60
1:A:455:ALA:CB	1:A:469:LEU:HD11	2.31	0.60
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.37	0.60
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:90:VAL:HG12	5:A:2033:HOH:O	2.03	0.58
2:B:88:TRP:C	2:B:90:VAL:H	2.05	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:142:ILE:HD13	2:B:142:ILE:N	2.21	0.56
2:B:6:GLU:HA	5:B:2001:HOH:O	2.06	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: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:420:PRO:O	2:B:420:PRO:HD2	2.07	0.54
2:B:126:LYS:HA	2:B:145:GLN:OE1	2.08	0.54
2:B:243:PRO:O	2:B:244:ILE:C	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.47	0.53
2:B:286:THR:O	2:B:286:THR:HG22	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: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
1:A:64:LYS:HD2	1:A:69:THR:HA	1.91	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:295:LEU:O	2:B:296:THR:OG1	2.26	0.51
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.98	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:163:SER:O	2:B:167:ILE:HG13	2.10	0.51
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.93	0.51
1:A:89:GLU:HG2	1:A:91:GLN:CA	2.39	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:88:TRP:C	2:B:90:VAL:N	2.64	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
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.90	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
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:271:TYR:HB3	2:B:309:ILE:HD11	1.95	0.47
2:B:89:GLU:HA	2:B:93:GLY:CA	2.44	0.47
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.49	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
1:A:216:THR:O	1:A:218:ASP:N	2.48	0.47
2:B:334:GLN:HG3	2:B:334:GLN:O	2.15	0.47
2:B:33:ALA:O	2:B:37:ILE:HD12	2.15	0.47
1:A:243:PRO:CG	1:A:244:ILE:N	2.74	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
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:243:PRO:HG3	2:B:351:THR:HG1	1.80	0.46
2:B:394:GLN:HB3	2:B:397:THR:OG1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:TYR:HB3	2:B:149:LEU:HB2	1.97	0.46
2:B:11:LYS:HD2	2:B:11:LYS:HA	1.85	0.46
2:B:260:LEU:O	2:B:260:LEU:HD13	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
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:308:GLU:HA	1:A:308:GLU:OE1	2.17	0.44
1:A:3:SER:HB3	1:A:5:ILE:HG22	1.98	0.44
1:A:89:GLU:C	1:A:91:GLN:H	2.19	0.44
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.83	0.44
2:B:297:GLU:CG	2:B:298:GLU:H	2.30	0.44
2:B:53:GLU:OE1	2:B:53:GLU:N	2.43	0.44
1:A:107:THR:HG22	1:A:198:HIS:NE2	2.33	0.44
2:B:248:GLU:C	2:B:250:ASP:H	2.20	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
2:B:155:GLY:O	2:B:159:ILE:HG12	2.18	0.43
1:A:39:THR:O	1:A:40:GLU:C	2.57	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
2:B:164:MET:HE1	2:B:209:LEU:HD21	1.99	0.43
1:A:379:SER:CB	1:A:387:PRO:HD3	2.49	0.43
1:A:224:GLU:HA	1:A:225:PRO:HD2	1.74	0.43
1:A:61:PHE:HE2	1:A:74:LEU:HD12	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HE2	1:A:284:ARG:HH22	1.84	0.43
1:A:95:PRO:HB3	2:B:136:ASN:ND2	2.34	0.43
1:A:537:PRO:HD2	1:A:542:ILE:HD13	2.01	0.42
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.54	0.42
1:A:24:TRP:HH2	1:A:61:PHE:CD1	2.37	0.42
2:B:121:ASP:C	2:B:121:ASP:OD1	2.58	0.42
2:B:366:LYS:HB3	5:B:2098:HOH:O	2.18	0.42
2:B:328:GLU:CG	2:B:390:LYS:HD3	2.49	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
1:A:136:ASN:O	1:A:137:ASN:C	2.58	0.42
1:A:28:GLU:O	1:A:29:GLU:C	2.57	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:156:SER:N	1:A:157:PRO:CD	2.83	0.42
1:A:89:GLU:HA	1:A:92:LEU:HD13	2.01	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
2:B:241:VAL:HG22	2:B:243:PRO:HD3	2.01	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.21	0.41
2:B:30:LYS:O	2:B:34:LEU:HB2	2.21	0.41
1:A:10:VAL:HG22	1:A:124:PHE:CD1	2.55	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
2:B:47:ILE:HD12	2:B:144:TYR:CG	2.56	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
1:A:89:GLU:HB3	1:A:90:VAL:H	1.73	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:HD22	1:A:422:LEU:H	1.85	0.40
1:A:467:VAL:HA	1:A:468:PRO:HD2	1.97	0.40
1:A:77:PHE:O	1:A:78:ARG:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:O	1:A:56:TYR:CB	2.69	0.40
1:A:148:VAL:O	1:A:150:PRO:HD3	2.22	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
1:A:54:ASN:HD21	1:A:56:TYR:HD2	1.68	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%)	3 11
2	B	406/428 (95%)	352 (87%)	39 (10%)	15 (4%)	3 13
All	All	963/990 (97%)	841 (87%)	84 (9%)	38 (4%)	3 12

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	493/502 (98%)	428 (87%)	65 (13%)	4 12
2	B	373/390 (96%)	330 (88%)	43 (12%)	5 17
All	All	866/892 (97%)	758 (88%)	108 (12%)	4 14

All (108) 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	100	LEU
1	A	105	SER
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	221	HIS
1	A	222	GLN
1	A	223	LYS
1	A	238	LYS
1	A	248	GLU
1	A	249	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	LEU
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	317	VAL
1	A	321	PRO
1	A	323	LYS
1	A	332	GLN
1	A	349	LEU
1	A	357	MET
1	A	404	GLU
1	A	406	TRP
1	A	422	LEU
1	A	428	GLN
1	A	459	THR
1	A	467	VAL
1	A	479	LEU
1	A	484	LEU
1	A	500	GLN
1	A	507	GLN
1	A	512	LYS
1	A	517	LEU
1	A	527	LYS
1	A	530	LYS
1	A	533	LEU
1	A	540	LYS
1	A	548	VAL
1	A	550	LYS
2	B	3	SER
2	B	5	ILE
2	B	6	GLU
2	B	34	LEU
2	B	67	ASP
2	B	83	ARG
2	B	90	VAL
2	B	117	SER
2	B	139	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	175	ASN
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	298	GLU
2	B	301	LEU
2	B	309	ILE
2	B	317	VAL
2	B	326	ILE
2	B	336	GLN
2	B	344	GLU
2	B	345	PRO
2	B	347	LYS
2	B	356	ARG
2	B	363	ASN
2	B	387	PRO
2	B	399	GLU
2	B	410	TRP
2	B	414	TRP
2	B	419	THR
2	B	422	LEU
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	151	GLN
1	A	161	GLN
1	A	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	361	HIS
1	A	367	GLN
1	A	474	ASN
1	A	494	ASN
2	B	57	ASN
2	B	85	GLN
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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	16,22,22	1.70	2 (12%)	19,32,32	1.98	5 (26%)

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	-	-	0/0/11/11	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1559	YKN	C13-S12	-5.44	1.67	1.76
3	A	1559	YKN	F10-C9	-2.38	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1559	YKN	C13-N15-C16	4.25	120.63	115.96
3	A	1559	YKN	N20-C13-N15	-4.02	122.58	127.57
3	A	1559	YKN	C18-C19-N20	-2.99	120.25	123.96
3	A	1559	YKN	F11-C9-F10	-2.95	102.96	107.34
3	A	1559	YKN	C19-N20-C13	2.72	119.02	114.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

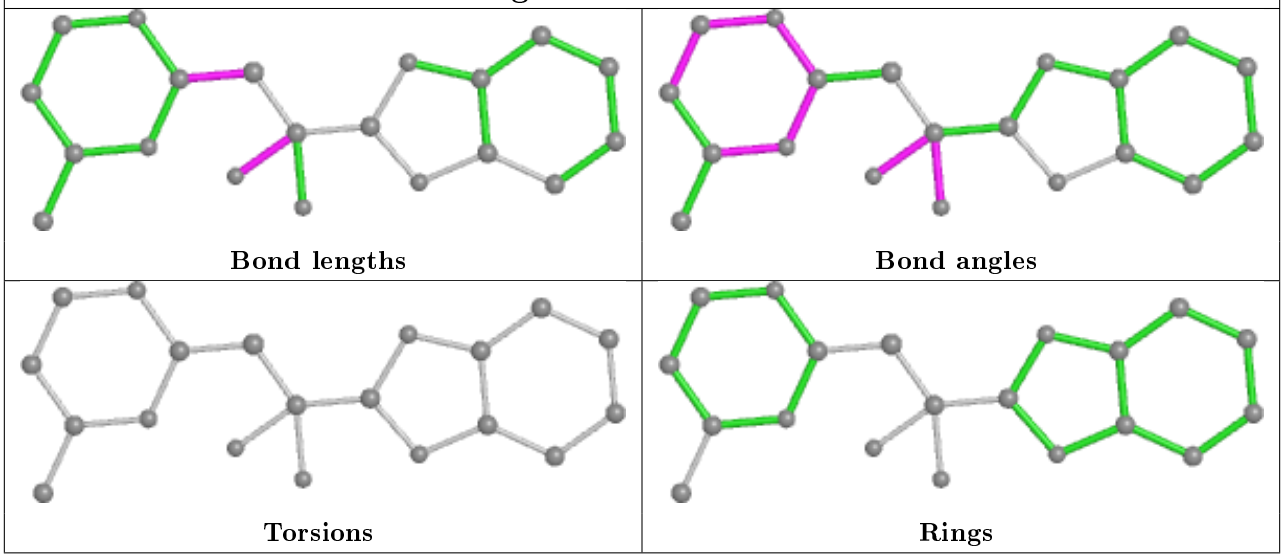
1 monomer is involved in 1 short contact:

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand YKN A 1559



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

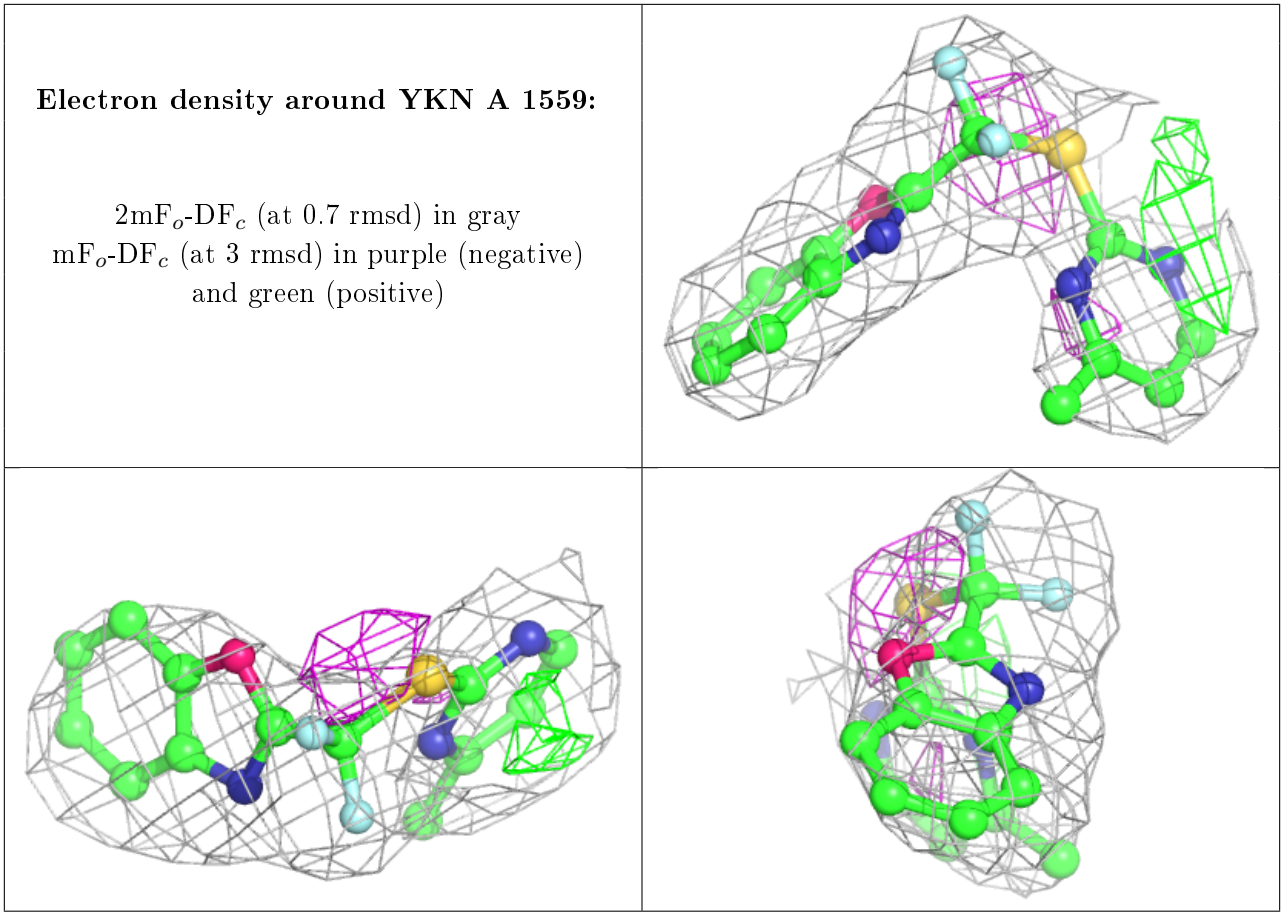
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 YKN A 1559:

$2mF_o$-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

Unable to reproduce the depositors R factor - this section is therefore empty.