Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 10:11 am BST

PDB ID	:	2YKN
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	:	2.12 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 (i) 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 (i)) were used in the production of this report:

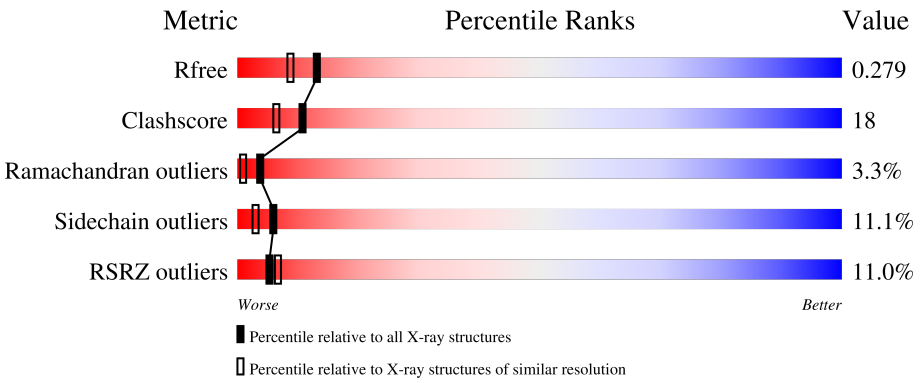
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 <=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	9% 68% 23% 7% ••
2	B	428	13% 64% 23% 8% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8192 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
			Total	C	N	O	S			
1	A	558	4506	2917	746	835	8	0	1	1

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	LEU	PHE	engineered mutation	UNP P03366
A	478	GLN	GLU	engineered mutation	UNP P03366

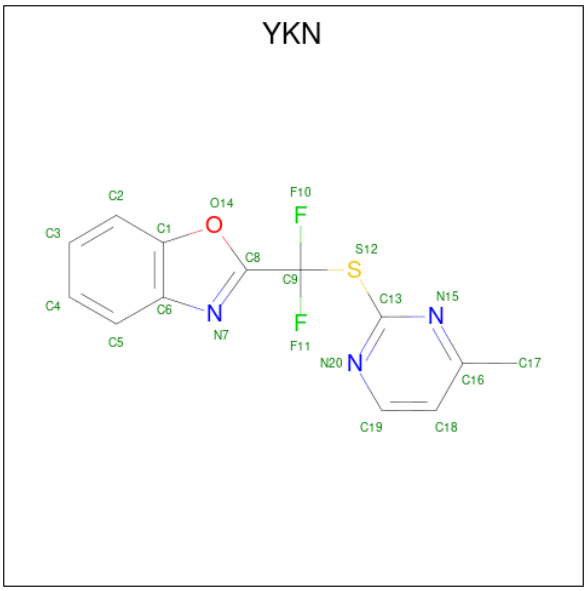
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

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

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
			Total	C	F	N	O	S		
3	A	1	20	13	2	3	1	1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

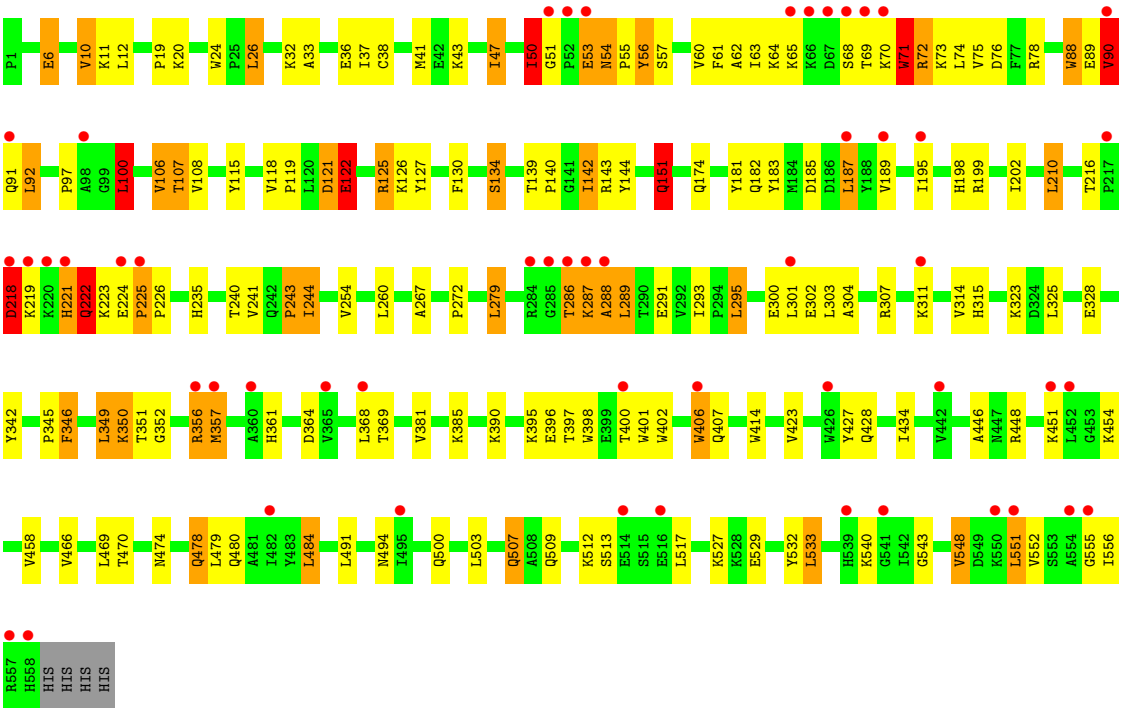
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	162	162	162	0	0
			Total	O		
5	B	114	114	114	0	0

3 Residue-property plots (i)

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.

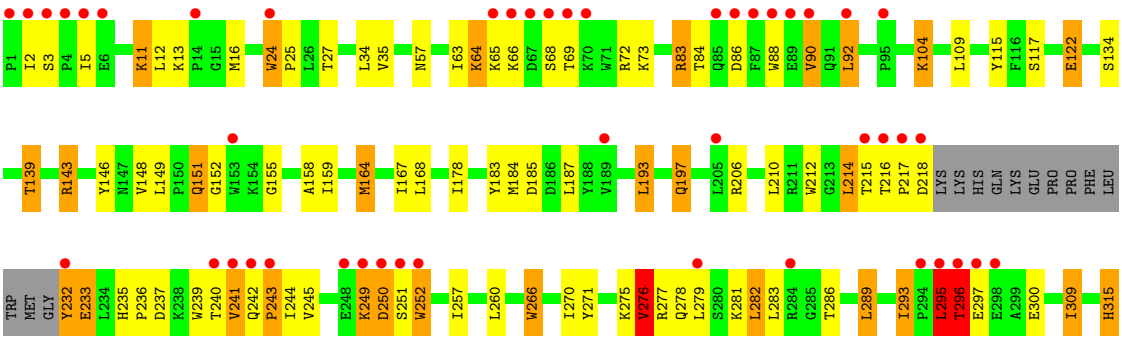
• Molecule 1: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

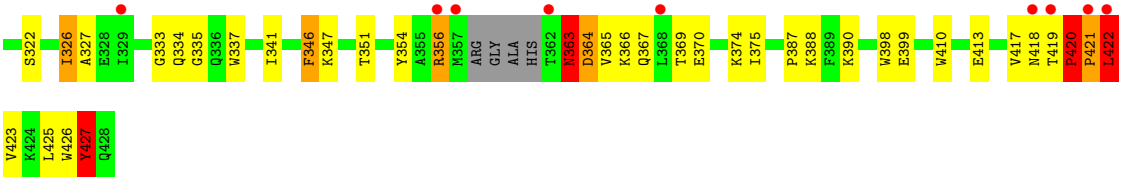
Chain A:



• Molecule 2: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

Chain B:




S322
I326
A327
E328
I329
G333
Q334
G335
Q336
W337
I341
F346
K347
T351
Y354
A355
R356
M357
ARG
GLY
ALA
HIS
T362
N363
D364
V365
K366
Q367
L368
T369
E370
K374
I375
P387
K388
F389
K390
W398
E399
W410
E413
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 – 2.12 19.45 – 2.12	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-2.12) 92.6 (19.45-2.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.279 0.227 , 0.279	Depositor DCC
R_{free} test set	3764 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8192	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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 (i)

5.1 Standard geometry (i)

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	1.07	10/4626 (0.2%)	1.00	18/6289 (0.3%)
2	B	1.05	5/3490 (0.1%)	1.14	8/4747 (0.2%)
All	All	1.06	15/8116 (0.2%)	1.06	26/11036 (0.2%)

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	1	1
2	B	0	3
All	All	1	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	VAL	CB-CG2	7.41	1.68	1.52
2	B	143	ARG	CG-CD	-6.98	1.34	1.51
1	A	10	VAL	CB-CG1	-6.42	1.39	1.52
2	B	148	VAL	CB-CG1	6.10	1.65	1.52
1	A	57	SER	CB-OG	6.01	1.50	1.42
2	B	152	GLY	N-CA	5.93	1.54	1.46
1	A	6	GLU	CG-CD	5.89	1.60	1.51
1	A	185	ASP	CB-CG	-5.83	1.39	1.51
2	B	266	TRP	CB-CG	-5.70	1.40	1.50
1	A	122	GLU	N-CA	5.70	1.57	1.46
1	A	134	SER	CB-OG	-5.45	1.35	1.42
1	A	396	GLU	CG-CD	5.17	1.59	1.51
2	B	427	TYR	C-N	-5.15	1.22	1.34
1	A	115	TYR	CD2-CE2	5.10	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	PHE	N-CA	-5.00	1.36	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	427	TYR	O-C-N	-32.69	70.40	122.70
2	B	427	TYR	CA-C-O	-18.30	81.67	120.10
2	B	427	TYR	CA-C-N	15.84	152.04	117.20
1	A	185	ASP	CB-CG-OD1	-10.45	108.90	118.30
1	A	345	PRO	C-N-CA	7.60	140.70	121.70
1	A	151	GLN	C-N-CA	-7.30	106.98	122.30
2	B	151	GLN	C-N-CA	-6.99	107.62	122.30
1	A	484	LEU	CA-CB-CG	6.56	130.40	115.30
1	A	187	LEU	CB-CG-CD1	6.54	122.12	111.00
1	A	346	PHE	CB-CA-C	6.31	123.03	110.40
1	A	108	VAL	CB-CA-C	-6.22	99.58	111.40
1	A	100	LEU	CB-CG-CD1	6.06	121.30	111.00
1	A	345	PRO	O-C-N	5.82	132.02	122.70
2	B	143	ARG	CA-CB-CG	-5.77	100.70	113.40
1	A	143	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	345	PRO	CA-C-N	-5.69	104.69	117.20
2	B	252	TRP	CA-CB-CG	5.62	124.37	113.70
1	A	121	ASP	C-N-CA	-5.48	108.01	121.70
1	A	125	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	26	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	533	LEU	CB-CG-CD2	5.34	120.07	111.00
2	B	143	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	185	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	346	PHE	N-CA-C	5.09	124.75	111.00
2	B	164	MET	CG-SD-CE	5.07	108.31	100.20
1	A	50	ILE	CG1-CB-CG2	5.03	122.47	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	346	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TRP	Peptide
2	B	295	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	417	VAL	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	4506	0	4554	168	0
2	B	3389	0	3416	134	0
3	A	20	0	9	0	0
4	A	1	0	0	0	0
5	A	162	0	0	9	0
5	B	114	0	0	6	0
All	All	8192	0	7979	291	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 18.

All (291) 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:89:GLU:CG	1:A:90:VAL:H	1.28	1.30
2:B:266:TRP:HH2	2:B:427:TYR:OH	1.20	1.20
1:A:107:THR:HG21	1:A:202:ILE:CD1	1.73	1.17
1:A:89:GLU:HG2	1:A:90:VAL:N	1.49	1.12
2:B:271:TYR:HB3	2:B:309:ILE:HD11	1.25	1.12
2:B:420:PRO:O	2:B:421:PRO:O	1.68	1.11
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.12	1.09
1:A:121:ASP:O	1:A:122:GLU:CB	1.93	1.08
1:A:107:THR:HG21	1:A:202:ILE:HD11	1.37	1.06
2:B:249:LYS:HB2	2:B:252:TRP:HE1	1.21	1.05
2:B:249:LYS:HB2	2:B:252:TRP:NE1	1.71	1.05
2:B:281:LYS:O	2:B:282:LEU:HB2	1.51	1.05
2:B:13:LYS:CD	2:B:86:ASP:HB2	1.88	1.01
1:A:434:ILE:H	1:A:494:ASN:HD21	1.09	1.01
5:A:2134:HOH:O	2:B:363:ASN:O	1.78	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:O	1:A:90:VAL:HG22	1.60	1.01
2:B:13:LYS:HD2	2:B:86:ASP:CB	1.90	1.00
2:B:363:ASN:HD21	2:B:365:VAL:HG12	1.25	0.98
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.47	0.96
1:A:54:ASN:ND2	1:A:55:PRO:O	2.01	0.94
1:A:451:LYS:O	1:A:470:THR:O	1.87	0.91
2:B:13:LYS:HD2	2:B:86:ASP:HB2	0.94	0.91
1:A:121:ASP:O	1:A:122:GLU:HB2	1.71	0.91
1:A:89:GLU:CG	1:A:90:VAL:N	2.07	0.90
1:A:121:ASP:O	1:A:122:GLU:HB3	1.70	0.90
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.51	0.89
2:B:241:VAL:HG13	2:B:242:GLN:H	1.40	0.87
2:B:282:LEU:HD21	2:B:295:LEU:HB3	1.55	0.86
1:A:89:GLU:HG2	1:A:90:VAL:H	0.70	0.86
2:B:281:LYS:O	2:B:282:LEU:CB	2.22	0.86
1:A:243:PRO:HD2	1:A:244:ILE:HG13	1.57	0.85
1:A:325:LEU:HD23	1:A:385:LYS:HE2	1.56	0.85
2:B:420:PRO:O	2:B:421:PRO:C	2.12	0.84
1:A:240:THR:HG22	1:A:241:VAL:H	1.42	0.84
1:A:325:LEU:CD2	1:A:385:LYS:HE2	2.08	0.83
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.67	0.82
2:B:282:LEU:CD2	2:B:295:LEU:HB3	2.10	0.81
1:A:107:THR:CG2	1:A:202:ILE:HD11	2.11	0.79
1:A:361:HIS:HD2	1:A:513:SER:OG	1.66	0.79
1:A:63:ILE:HG13	1:A:64:LYS:N	1.97	0.79
2:B:363:ASN:ND2	2:B:365:VAL:HG12	1.97	0.78
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.30	0.77
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.02	0.77
2:B:232:TYR:HD1	2:B:233:GLU:H	1.33	0.77
2:B:122:GLU:CD	2:B:122:GLU:H	1.89	0.75
2:B:164:MET:CE	2:B:187:LEU:HD11	2.17	0.74
2:B:356:ARG:HH11	2:B:356:ARG:CG	1.97	0.74
2:B:356:ARG:HG2	2:B:356:ARG:NH1	1.92	0.74
2:B:249:LYS:HB2	2:B:252:TRP:CD1	2.22	0.74
1:A:507:GLN:O	1:A:509[B]:GLN:NE2	2.21	0.73
2:B:24[B]:TRP:CH2	2:B:399:GLU:OE1	2.41	0.73
1:A:63:ILE:HG13	1:A:64:LYS:H	1.52	0.73
2:B:232:TYR:O	2:B:233:GLU:HB2	1.88	0.73
2:B:164:MET:HE1	2:B:187:LEU:HD11	1.69	0.73
1:A:494:ASN:HD22	1:A:532:TYR:HB3	1.54	0.72
1:A:63:ILE:HG23	1:A:65:LYS:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD23	1:A:385:LYS:CE	2.21	0.70
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.73	0.70
1:A:134:SER:OG	1:A:139:THR:HG22	1.91	0.70
1:A:357:MET:SD	1:A:357:MET:N	2.64	0.70
2:B:295:LEU:O	2:B:296:THR:OG1	2.08	0.70
2:B:420:PRO:C	2:B:421:PRO:O	2.29	0.70
1:A:361:HIS:CD2	1:A:513:SER:OG	2.45	0.69
1:A:97:PRO:HA	1:A:100:LEU:HD22	1.73	0.69
2:B:249:LYS:CB	2:B:252:TRP:HE1	2.03	0.69
1:A:12:LEU:HD21	1:A:127:TYR:CE2	2.28	0.69
2:B:257:ILE:HD11	2:B:293:ILE:HG13	1.75	0.69
2:B:364:ASP:N	5:B:2106:HOH:O	1.70	0.69
1:A:89:GLU:O	1:A:90:VAL:CG2	2.37	0.68
1:A:351:THR:HG22	1:A:352:GLY:N	2.08	0.68
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.30	0.67
1:A:406:TRP:CD2	2:B:420:PRO:HG3	2.29	0.67
1:A:218:ASP:HB2	1:A:222:GLN:HB2	1.77	0.67
1:A:54:ASN:C	1:A:54:ASN:HD22	1.99	0.66
2:B:356:ARG:HD3	2:B:367:GLN:HG2	1.78	0.66
1:A:235:HIS:ND1	5:A:2090:HOH:O	2.30	0.65
1:A:369:THR:OG1	1:A:398:TRP:HZ3	1.80	0.65
2:B:250:ASP:CG	2:B:251:SER:N	2.49	0.65
2:B:206:ARG:HD3	2:B:217:PRO:O	1.96	0.65
1:A:406:TRP:HE3	1:A:407:GLN:HE21	1.45	0.65
1:A:434:ILE:H	1:A:494:ASN:ND2	1.87	0.65
1:A:92:LEU:HD23	1:A:92:LEU:C	2.17	0.64
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.44	0.63
2:B:293:ILE:HD13	2:B:293:ILE:O	1.99	0.63
1:A:434:ILE:N	1:A:494:ASN:HD21	1.89	0.62
1:A:216:THR:HB	1:A:218:ASP:OD1	1.99	0.62
1:A:70:LYS:O	1:A:71:TRP:HB2	1.97	0.62
2:B:354:TYR:OH	2:B:370:GLU:OE1	2.15	0.61
1:A:89:GLU:C	1:A:90:VAL:HG22	2.19	0.61
2:B:363:ASN:HB3	5:B:2106:HOH:O	1.99	0.61
2:B:363:ASN:O	2:B:364:ASP:HB2	1.98	0.61
1:A:356:ARG:HA	1:A:357:MET:SD	2.41	0.61
1:A:139:THR:OG1	1:A:140:PRO:CD	2.49	0.61
1:A:90:VAL:HG13	5:A:2037:HOH:O	2.00	0.60
1:A:19:PRO:O	1:A:56:TYR:HA	2.02	0.60
1:A:182:GLN:HB3	5:A:2078:HOH:O	2.01	0.60
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:O	1:A:37:ILE:HG12	2.02	0.60
2:B:243:PRO:HG3	2:B:351:THR:OG1	2.01	0.60
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.65	0.59
1:A:64:LYS:NZ	1:A:69:THR:HA	2.17	0.59
1:A:503:LEU:CD2	2:B:422:LEU:HD12	2.33	0.59
1:A:406:TRP:CE3	2:B:420:PRO:HG3	2.37	0.59
1:A:63:ILE:CG1	1:A:64:LYS:H	2.16	0.58
1:A:122:GLU:CA	1:A:125:ARG:HG3	2.28	0.58
2:B:249:LYS:CB	2:B:252:TRP:NE1	2.59	0.58
1:A:142:ILE:CD1	1:A:142:ILE:N	2.66	0.58
1:A:61:PHE:CE2	1:A:74:LEU:HD12	2.38	0.58
2:B:35:VAL:HG23	5:B:2013:HOH:O	2.04	0.58
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.86	0.58
1:A:287:LYS:HB3	1:A:291:GLU:OE2	2.04	0.57
2:B:354:TYR:CD1	2:B:374:LYS:HD3	2.40	0.57
1:A:240:THR:HG22	1:A:241:VAL:N	2.17	0.57
1:A:406:TRP:CZ3	2:B:418:ASN:O	2.58	0.57
2:B:109:LEU:HA	2:B:218:ASP:HA	1.87	0.57
1:A:139:THR:OG1	1:A:140:PRO:HD2	2.04	0.57
2:B:388:LYS:HG2	2:B:413:GLU:HB2	1.85	0.57
1:A:55:PRO:O	1:A:56:TYR:CB	2.49	0.56
1:A:92:LEU:HD23	1:A:92:LEU:O	2.04	0.56
1:A:351:THR:CG2	1:A:352:GLY:N	2.68	0.56
2:B:249:LYS:HD2	2:B:252:TRP:HD1	1.71	0.55
1:A:63:ILE:CG1	1:A:64:LYS:N	2.67	0.55
2:B:363:ASN:HB3	2:B:366:LYS:HB3	1.87	0.55
2:B:214:LEU:HD13	2:B:215:THR:H	1.71	0.55
1:A:142:ILE:N	1:A:142:ILE:HD13	2.21	0.55
1:A:122:GLU:HA	1:A:125:ARG:CG	2.28	0.55
2:B:266:TRP:CH2	2:B:427:TYR:OH	2.11	0.55
1:A:76:ASP:OD1	1:A:78:ARG:HG2	2.07	0.55
1:A:202:ILE:HG21	1:A:221:HIS:HB3	1.89	0.54
1:A:63:ILE:CG2	1:A:65:LYS:HG2	2.38	0.54
2:B:206:ARG:HG2	2:B:217:PRO:HD2	1.88	0.54
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.90	0.53
2:B:88:TRP:N	2:B:88:TRP:CD1	2.73	0.53
2:B:363:ASN:CA	5:B:2106:HOH:O	2.56	0.53
2:B:241:VAL:CG1	2:B:242:GLN:H	2.17	0.53
1:A:89:GLU:HG3	1:A:90:VAL:H	1.52	0.53
1:A:151:GLN:H	1:A:151:GLN:NE2	2.06	0.53
1:A:548:VAL:O	1:A:552:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.43	0.53
2:B:354:TYR:HD1	2:B:374:LYS:HD3	1.73	0.53
1:A:43:LYS:HG2	5:A:2024:HOH:O	2.08	0.53
1:A:287:LYS:O	1:A:288:ALA:CB	2.56	0.53
2:B:363:ASN:HD21	2:B:365:VAL:CG1	2.10	0.53
1:A:543:GLY:HA3	2:B:283:LEU:O	2.08	0.53
2:B:250:ASP:OD1	2:B:251:SER:N	2.42	0.52
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.25	0.52
1:A:235:HIS:CE1	5:A:2090:HOH:O	2.61	0.52
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.53	0.52
1:A:243:PRO:CD	1:A:244:ILE:HG13	2.35	0.52
2:B:420:PRO:O	2:B:420:PRO:HG2	2.09	0.52
1:A:325:LEU:CD2	1:A:385:LYS:CE	2.83	0.52
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.91	0.52
1:A:106:VAL:HA	1:A:189:VAL:O	2.10	0.51
2:B:104:LYS:O	2:B:235:HIS:HD2	1.93	0.51
2:B:155:GLY:O	2:B:159:ILE:HG12	2.10	0.51
1:A:218:ASP:CB	1:A:222:GLN:HB2	2.40	0.51
1:A:38:CYS:HA	1:A:41:MET:CE	2.41	0.51
2:B:326:ILE:HD13	2:B:390:LYS:HD2	1.93	0.51
1:A:41:MET:HE1	1:A:73:LYS:CD	2.42	0.50
1:A:279:LEU:HD22	1:A:302:GLU:OE1	2.11	0.50
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.45	0.50
1:A:90:VAL:HG12	5:A:2030:HOH:O	2.10	0.50
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.42	0.50
2:B:286:THR:HG22	2:B:286:THR:O	2.11	0.50
1:A:134:SER:HB2	1:A:139:THR:O	2.11	0.50
1:A:406:TRP:CE2	2:B:420:PRO:HG3	2.47	0.50
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.43	0.50
2:B:24[A]:TRP:HA	2:B:24[A]:TRP:CE3	2.47	0.49
2:B:151:GLN:O	2:B:185:ASP:OD1	2.30	0.49
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.94	0.49
1:A:55:PRO:O	1:A:56:TYR:HB2	2.13	0.49
2:B:164:MET:HE2	2:B:187:LEU:HD11	1.94	0.49
2:B:296:THR:HG22	2:B:300:GLU:HG2	1.94	0.49
2:B:297:GLU:HA	2:B:300:GLU:HG3	1.95	0.49
1:A:195:ILE:HG22	1:A:199:ARG:CZ	2.43	0.49
1:A:427:TYR:CE2	1:A:509[B]:GLN:HG3	2.48	0.49
2:B:11:LYS:HG3	2:B:12:LEU:O	2.13	0.49
1:A:474:ASN:O	1:A:478:GLN:HG2	2.13	0.48
2:B:346:PHE:N	2:B:346:PHE:CD1	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:MET:HE3	2:B:168:LEU:HD21	1.95	0.48
2:B:335:GLY:HA2	2:B:367:GLN:HE22	1.78	0.48
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.96	0.48
1:A:11:LYS:HE3	1:A:12:LEU:O	2.13	0.48
2:B:206:ARG:CG	2:B:217:PRO:HD2	2.43	0.48
2:B:363:ASN:CB	5:B:2106:HOH:O	2.60	0.48
2:B:64:LYS:HD3	2:B:68:SER:H	1.78	0.48
2:B:356:ARG:CD	2:B:367:GLN:HG2	2.44	0.48
1:A:92:LEU:N	1:A:92:LEU:HD22	2.29	0.48
2:B:249:LYS:HD2	2:B:252:TRP:CD1	2.49	0.48
2:B:333:GLY:O	2:B:334:GLN:HB3	2.14	0.48
1:A:454:LYS:NZ	1:A:555:GLY:HA3	2.30	0.47
2:B:232:TYR:HD1	2:B:233:GLU:N	2.08	0.47
1:A:243:PRO:CG	1:A:244:ILE:N	2.77	0.47
2:B:275:LYS:O	2:B:276:VAL:CB	2.58	0.47
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.48	0.47
2:B:35:VAL:CG2	5:B:2013:HOH:O	2.63	0.47
2:B:266:TRP:CG	2:B:426:TRP:CD1	3.03	0.47
1:A:240:THR:OG1	1:A:315:HIS:ND1	2.47	0.47
1:A:92:LEU:HD22	1:A:92:LEU:H	1.80	0.47
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.96	0.47
1:A:406:TRP:HZ3	2:B:418:ASN:O	1.97	0.47
1:A:32:LYS:NZ	1:A:36:GLU:OE2	2.48	0.46
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.96	0.46
2:B:326:ILE:CD1	2:B:390:LYS:HD2	2.44	0.46
1:A:38:CYS:HA	1:A:41:MET:HE3	1.97	0.46
1:A:89:GLU:HG2	1:A:90:VAL:CA	2.39	0.46
1:A:20:LYS:HG2	1:A:56:TYR:H	1.80	0.46
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.50	0.46
1:A:446:ALA:H	1:A:474:ASN:ND2	2.13	0.46
2:B:214:LEU:HD12	2:B:217:PRO:HG3	1.96	0.46
1:A:92:LEU:N	1:A:92:LEU:CD2	2.78	0.46
1:A:89:GLU:C	1:A:90:VAL:CG2	2.80	0.45
2:B:164:MET:HE2	2:B:168:LEU:HD11	1.98	0.45
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.98	0.45
1:A:50:ILE:HD13	1:A:51:GLY:H	1.80	0.45
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.98	0.45
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.76	0.45
1:A:397:THR:O	1:A:400:THR:HG22	2.17	0.45
2:B:65:LYS:O	2:B:66:LYS:HD3	2.16	0.45
2:B:337:TRP:HE1	2:B:367:GLN:NE2	2.06	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:CB	2:B:309:ILE:HD11	2.19	0.45
2:B:420:PRO:O	2:B:420:PRO:CG	2.62	0.45
1:A:454:LYS:CE	1:A:555:GLY:HA3	2.46	0.45
2:B:88:TRP:C	2:B:90:VAL:H	2.21	0.45
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.15	0.45
2:B:63:ILE:HD11	2:B:72:ARG:HD3	1.98	0.45
1:A:89:GLU:HG2	1:A:90:VAL:C	2.37	0.45
1:A:272:PRO:HA	1:A:351:THR:HG21	1.98	0.45
1:A:469:LEU:HD21	1:A:480:GLN:HG2	2.00	0.44
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.52	0.44
2:B:270:ILE:HG12	2:B:346:PHE:O	2.18	0.44
2:B:293:ILE:H	2:B:293:ILE:HD12	1.82	0.44
2:B:419:THR:HG22	2:B:421:PRO:HD3	2.00	0.44
2:B:260:LEU:C	2:B:260:LEU:HD13	2.38	0.44
2:B:326:ILE:HD12	2:B:327:ALA:N	2.33	0.44
2:B:295:LEU:HD13	2:B:297:GLU:N	2.32	0.44
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.36	0.44
1:A:64:LYS:HZ2	1:A:69:THR:HA	1.82	0.43
1:A:361:HIS:HD2	1:A:513:SER:CB	2.30	0.43
2:B:315:HIS:ND1	2:B:315:HIS:C	2.70	0.43
1:A:62:ALA:HA	1:A:72:ARG:O	2.18	0.43
2:B:365:VAL:O	2:B:369:THR:HG23	2.18	0.43
1:A:12:LEU:HD21	1:A:127:TYR:CZ	2.53	0.43
1:A:88:TRP:CE2	2:B:143:ARG:HD3	2.53	0.43
1:A:303:LEU:O	1:A:307:ARG:HG3	2.18	0.43
2:B:164:MET:CE	2:B:168:LEU:HD21	2.49	0.43
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.54	0.43
2:B:134:SER:HB3	2:B:139:THR:HG22	2.01	0.43
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.99	0.43
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.49	0.42
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.55	0.42
1:A:287:LYS:O	1:A:288:ALA:HB3	2.18	0.42
1:A:325:LEU:HD21	1:A:385:LYS:HE2	1.97	0.42
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.02	0.42
2:B:295:LEU:HD11	2:B:297:GLU:HG2	2.02	0.42
1:A:350:LYS:HB2	1:A:350:LYS:HE2	1.77	0.42
1:A:92:LEU:C	1:A:92:LEU:CD2	2.88	0.42
1:A:6:GLU:CD	1:A:6:GLU:H	2.23	0.42
1:A:60:VAL:HG12	1:A:75:VAL:HG22	2.01	0.42
1:A:64:LYS:H	1:A:64:LYS:HG2	1.62	0.42
1:A:240:THR:HG23	1:A:314:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD22	1:A:423:VAL:HG21	2.02	0.42
2:B:363:ASN:ND2	2:B:366:LYS:H	2.18	0.41
2:B:421:PRO:C	2:B:423:VAL:H	2.23	0.41
1:A:41:MET:HE1	1:A:73:LYS:HD2	2.02	0.41
1:A:89:GLU:O	1:A:90:VAL:CB	2.68	0.41
1:A:89:GLU:HG3	1:A:90:VAL:N	2.20	0.41
1:A:301:LEU:O	1:A:304:ALA:HB3	2.20	0.41
1:A:491:LEU:HB3	1:A:529:GLU:HG3	2.02	0.41
2:B:84:THR:O	2:B:84:THR:HG22	2.20	0.41
1:A:53:GLU:H	1:A:53:GLU:HG3	1.37	0.41
2:B:214:LEU:HD13	2:B:215:THR:N	2.35	0.41
2:B:275:LYS:O	2:B:276:VAL:HB	2.18	0.41
1:A:243:PRO:HB2	1:A:244:ILE:H	1.48	0.41
1:A:351:THR:HG23	5:A:2107:HOH:O	2.20	0.41
1:A:12:LEU:CD2	1:A:127:TYR:CE2	3.02	0.41
1:A:202:ILE:HG21	1:A:221:HIS:CG	2.56	0.41
1:A:243:PRO:HD2	1:A:244:ILE:CG1	2.38	0.41
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.51	0.41
2:B:16:MET:CE	2:B:83:ARG:HG3	2.51	0.41
1:A:47:ILE:HG23	1:A:144:TYR:CD1	2.56	0.41
1:A:381:VAL:HG22	2:B:25:PRO:HG2	2.03	0.41
1:A:60:VAL:HG13	1:A:130:PHE:HB2	2.03	0.40
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.56	0.40
1:A:295:LEU:HB3	1:A:300:GLU:HG2	2.03	0.40
2:B:283:LEU:HD23	2:B:283:LEU:HA	1.91	0.40
1:A:126:LYS:HE3	5:A:2055:HOH:O	2.20	0.40
1:A:225:PRO:HB2	1:A:226:PRO:HD3	2.04	0.40
1:A:240:THR:CG2	1:A:241:VAL:H	2.23	0.40
2:B:210:LEU:HA	2:B:214:LEU:O	2.21	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%)	507 (91%)	32 (6%)	18 (3%)	4 1
2	B	406/428 (95%)	375 (92%)	17 (4%)	14 (3%)	3 1
All	All	963/990 (97%)	882 (92%)	49 (5%)	32 (3%)	4 1

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	122	GLU
1	A	218	ASP
1	A	222	GLN
1	A	243	PRO
1	A	288	ALA
1	A	311	LYS
1	A	356	ARG
1	A	556	ILE
2	B	2	ILE
2	B	233	GLU
2	B	243	PRO
2	B	276	VAL
2	B	363	ASN
2	B	364	ASP
2	B	420	PRO
2	B	421	PRO
1	A	91	GLN
1	A	223	LYS
1	A	225	PRO
1	A	244	ILE
1	A	286	THR
1	A	289	LEU
2	B	241	VAL
2	B	244	ILE
2	B	282	LEU
2	B	422	LEU
1	A	71	TRP
2	B	296	THR
1	A	448	ARG
2	B	69	THR
1	A	56	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	493/502 (98%)	443 (90%)	50 (10%)	7 4
2	B	373/390 (96%)	326 (87%)	47 (13%)	4 2
All	All	866/892 (97%)	769 (89%)	97 (11%)	6 3

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
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	68	SER
1	A	71	TRP
1	A	72	ARG
1	A	90	VAL
1	A	92	LEU
1	A	100	LEU
1	A	106	VAL
1	A	107	THR
1	A	142	ILE
1	A	151	GLN
1	A	174	GLN
1	A	187	LEU
1	A	210	LEU
1	A	218	ASP
1	A	219	LYS
1	A	221	HIS
1	A	222	GLN
1	A	224	GLU
1	A	260	LEU
1	A	279	LEU

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Mol	Chain	Res	Type
1	A	286	THR
1	A	287	LYS
1	A	289	LEU
1	A	295	LEU
1	A	323	LYS
1	A	346	PHE
1	A	349	LEU
1	A	350	LYS
1	A	357	MET
1	A	406	TRP
1	A	428	GLN
1	A	478	GLN
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	533	LEU
1	A	540	LYS
1	A	548	VAL
1	A	551	LEU
2	B	3	SER
2	B	5	ILE
2	B	11	LYS
2	B	24[A]	TRP
2	B	24[B]	TRP
2	B	27	THR
2	B	34	LEU
2	B	64	LYS
2	B	83	ARG
2	B	90	VAL
2	B	92	LEU
2	B	104	LYS
2	B	117	SER
2	B	122	GLU
2	B	139	THR
2	B	178	ILE
2	B	193	LEU
2	B	197	GLN
2	B	214	LEU

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Mol	Chain	Res	Type
2	B	216	THR
2	B	232	TYR
2	B	237	ASP
2	B	240	THR
2	B	245	VAL
2	B	249	LYS
2	B	250	ASP
2	B	276	VAL
2	B	277	ARG
2	B	278	GLN
2	B	279	LEU
2	B	289	LEU
2	B	293	ILE
2	B	295	LEU
2	B	296	THR
2	B	309	ILE
2	B	315	HIS
2	B	322	SER
2	B	326	ILE
2	B	346	PHE
2	B	347	LYS
2	B	356	ARG
2	B	363	ASN
2	B	387	PRO
2	B	410	TRP
2	B	420	PRO
2	B	422	LEU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	ASN
1	A	151	GLN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	221	HIS
1	A	255	ASN
1	A	361	HIS
1	A	367	GLN

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	474	ASN
1	A	494	ASN
1	A	507	GLN
2	B	57	ASN
2	B	147	ASN
2	B	161	GLN
2	B	235	HIS
2	B	242	GLN
2	B	258	GLN
2	B	278	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 monosaccharides 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	-	16,22,22	1.20	1 (6%)	19,32,32	2.87	7 (36%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1559	YKN	C13-S12	-3.10	1.71	1.76

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1559	YKN	C13-N15-C16	6.90	123.54	115.96
3	A	1559	YKN	N20-C13-N15	-6.37	119.67	127.57
3	A	1559	YKN	F10-C9-F11	-5.02	99.88	107.34
3	A	1559	YKN	C19-N20-C13	3.02	119.47	114.94
3	A	1559	YKN	C4-C3-C2	2.95	124.58	120.44
3	A	1559	YKN	C18-C16-N15	-2.21	118.52	121.55
3	A	1559	YKN	C3-C4-C5	-2.01	117.62	120.44

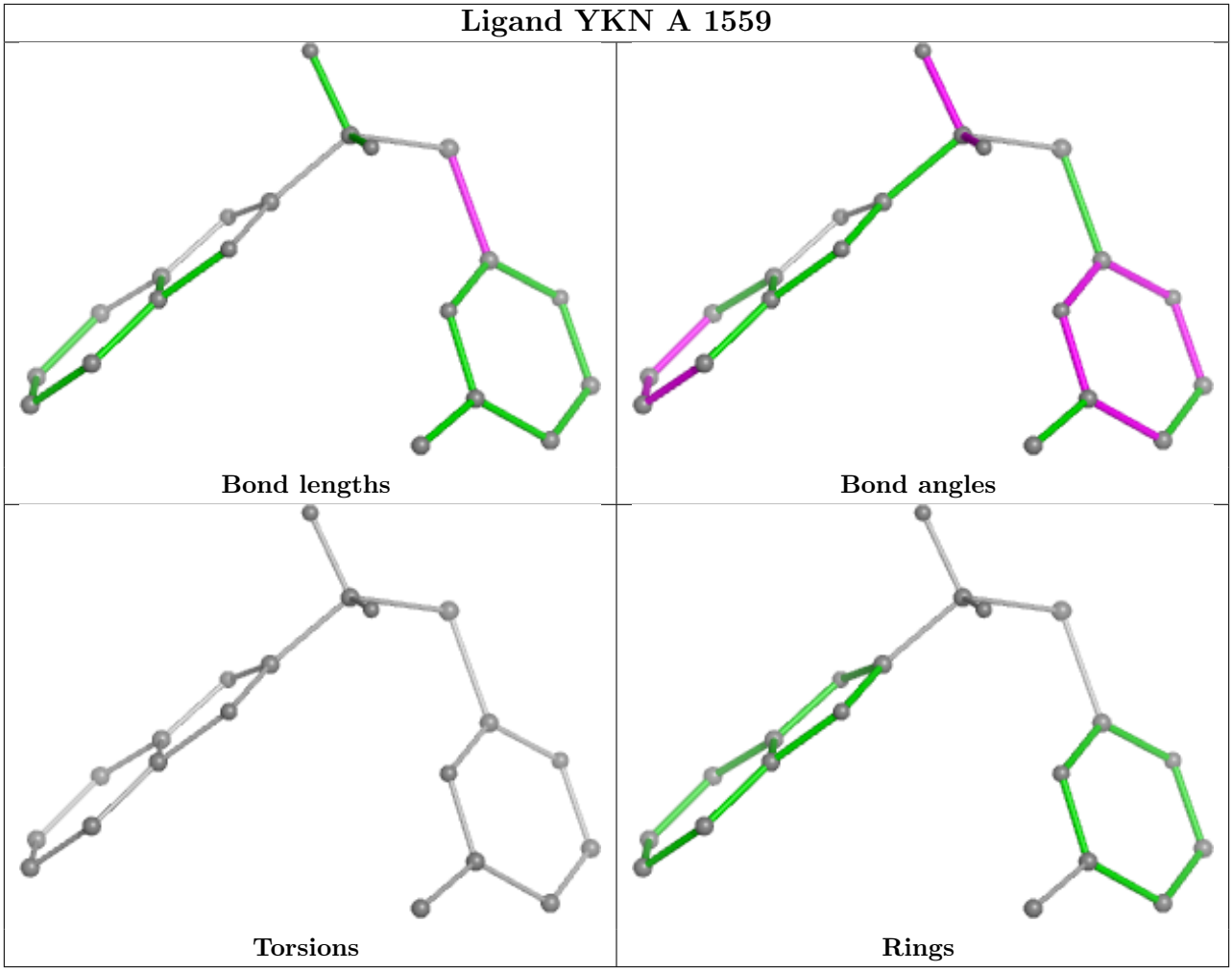
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	558/562 (99%)	0.45	52 (9%) 8 11	22, 38, 65, 83	0
2	B	411/428 (96%)	0.67	55 (13%) 3 4	21, 38, 73, 93	0
All	All	969/990 (97%)	0.54	107 (11%) 5 7	21, 38, 69, 93	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	294	PRO	12.3
2	B	216	THR	9.2
2	B	357	MET	8.8
2	B	2	ILE	8.6
2	B	295	LEU	8.6
2	B	3	SER	8.2
2	B	86	ASP	8.1
2	B	4	PRO	7.6
2	B	1	PRO	7.1
2	B	87	PHE	6.8
2	B	67	ASP	6.7
2	B	68	SER	6.4
1	A	286	THR	6.0
1	A	301	LEU	5.3
2	B	242	GLN	5.3
1	A	357	MET	5.1
2	B	69	THR	4.9
2	B	418	ASN	4.9
2	B	66	LYS	4.9
1	A	66	LYS	4.8
1	A	70	LYS	4.7
1	A	67	ASP	4.6
1	A	288	ALA	4.6
2	B	88	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	249	LYS	4.4
2	B	419	THR	4.2
1	A	68	SER	4.1
1	A	557	ARG	4.0
2	B	421	PRO	3.9
1	A	65	LYS	3.8
1	A	539	HIS	3.8
2	B	250	ASP	3.8
2	B	218	ASP	3.7
1	A	220	LYS	3.6
2	B	189	VAL	3.6
1	A	225	PRO	3.6
2	B	252	TRP	3.5
2	B	362	THR	3.5
1	A	221	HIS	3.5
2	B	5	ILE	3.4
2	B	251	SER	3.4
1	A	217	PRO	3.4
2	B	356	ARG	3.4
1	A	554	ALA	3.3
2	B	215	THR	3.3
1	A	51	GLY	3.3
1	A	287	LYS	3.2
2	B	241	VAL	3.1
1	A	558	HIS	3.1
1	A	555	GLY	3.0
2	B	90	VAL	3.0
1	A	541	GLY	3.0
2	B	296	THR	2.9
1	A	219	LYS	2.9
1	A	514	GLU	2.9
2	B	6	GLU	2.9
1	A	551	LEU	2.9
1	A	224	GLU	2.8
2	B	217	PRO	2.8
1	A	426	TRP	2.8
1	A	91	GLN	2.8
2	B	368	LEU	2.8
1	A	482	ILE	2.7
1	A	218	ASP	2.7
1	A	311	LYS	2.7
2	B	298	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	550	LYS	2.6
2	B	205	LEU	2.6
1	A	365	VAL	2.6
1	A	356	ARG	2.6
2	B	70	LYS	2.6
2	B	422	LEU	2.6
2	B	95	PRO	2.6
1	A	360	ALA	2.6
1	A	284	ARG	2.5
1	A	406	TRP	2.5
1	A	495	ILE	2.5
2	B	248	GLU	2.5
1	A	400	THR	2.5
2	B	279	LEU	2.5
1	A	285	GLY	2.5
1	A	98	ALA	2.5
2	B	284	ARG	2.4
2	B	232	TYR	2.4
1	A	189	VAL	2.4
1	A	90	VAL	2.4
1	A	69	THR	2.4
1	A	452	LEU	2.4
1	A	368	LEU	2.3
1	A	52	PRO	2.3
1	A	442	VAL	2.3
2	B	240	THR	2.3
2	B	92	LEU	2.3
2	B	89	GLU	2.3
1	A	53	GLU	2.3
1	A	187	LEU	2.2
2	B	24[A]	TRP	2.2
1	A	195	ILE	2.2
2	B	329	ILE	2.2
2	B	85	GLN	2.1
2	B	243	PRO	2.2
1	A	516	GLU	2.1
1	A	451	LYS	2.1
2	B	153	TRP	2.1
2	B	14	PRO	2.1
2	B	297	GLU	2.0
2	B	65	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

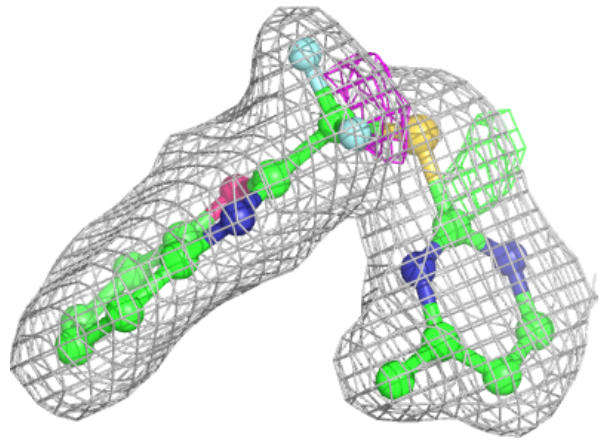
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

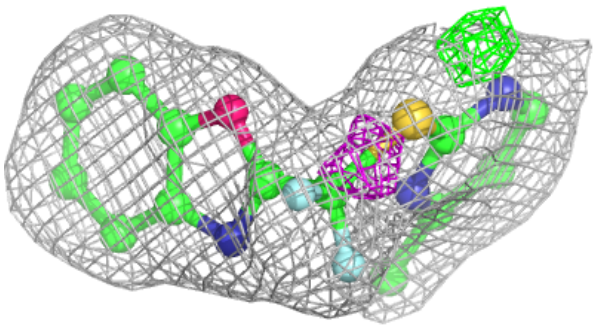
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	YKN	A	1559	20/20	0.90	0.15	28,35,46,50	0
4	CA	A	1560	1/1	0.92	0.12	73,73,73,73	0

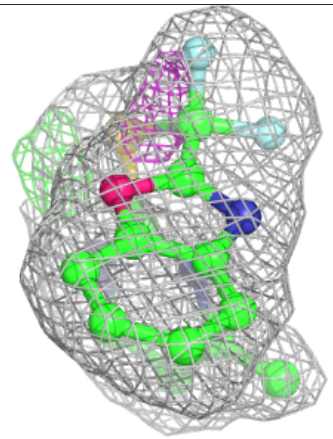
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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 (i)

There are no such residues in this entry.