Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 04:34 am GMT

PDB ID	:	2YNF
Title	:	HIV-1 Reverse Transcriptase Y188L mutant in complex with inhibitor GSK560
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Deposited on	:	2012-10-14
Resolution	:	2.36 Å(reported)

The following versions of software and data (see references ⓘ) 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
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

1 Overall quality at a glance ⓘ

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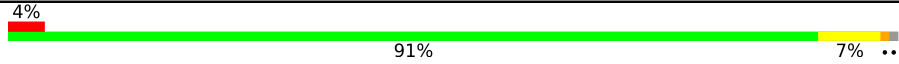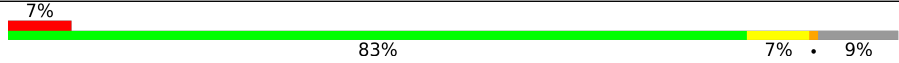*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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.
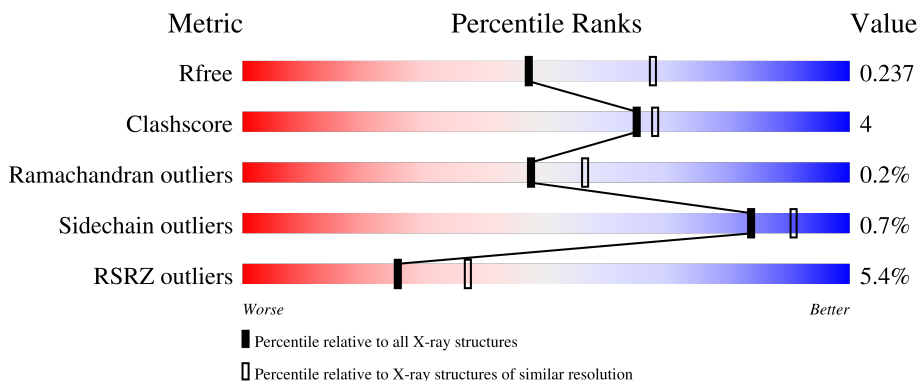
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	563	4% / 91% / 7% ..
2	B	447	7% / 83% / 7% . 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	1561	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8230 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	557	Total	C	N	O	S	0	2	0
			4463	2891	744	820	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P04585
A	-1	ASN	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	188	LEU	TYR	engineered mutation	UNP P04585

- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	2	0
			3291	2148	543	594	6			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	expression tag	UNP P04585
B	-17	ALA	-	expression tag	UNP P04585
B	-16	GLY	-	expression tag	UNP P04585
B	-15	HIS	-	expression tag	UNP P04585
B	-14	HIS	-	expression tag	UNP P04585
B	-13	HIS	-	expression tag	UNP P04585
B	-12	HIS	-	expression tag	UNP P04585
B	-11	HIS	-	expression tag	UNP P04585
B	-10	HIS	-	expression tag	UNP P04585
B	-9	GLY	-	expression tag	UNP P04585
B	-8	SER	-	expression tag	UNP P04585
B	-7	ALA	-	expression tag	UNP P04585

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLU	-	expression tag	UNP P04585
B	-5	ASN	-	expression tag	UNP P04585
B	-4	LEU	-	expression tag	UNP P04585
B	-3	TYR	-	expression tag	UNP P04585
B	-2	PHE	-	expression tag	UNP P04585
B	-1	GLN	-	expression tag	UNP P04585
B	0	GLY	-	expression tag	UNP P04585

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Mg 3	0	0

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).
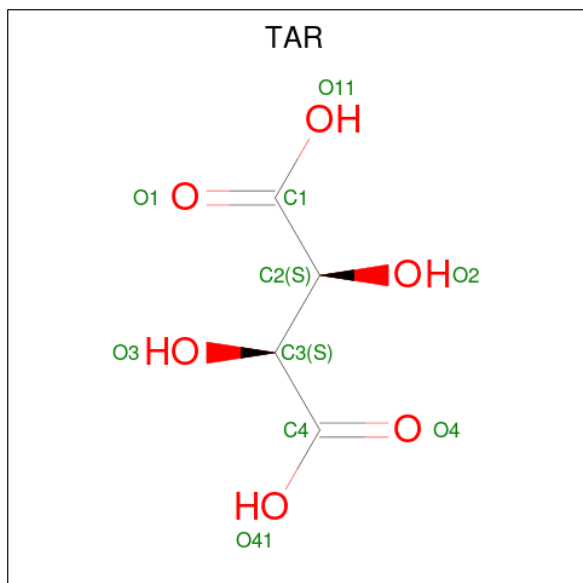
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 4	O 6	0	0

- Molecule 5 is 2-azanyl-N-[[4-bromanyl-3-(3-chloranyl-5-cyano-phenoxy)-2-fluoranyl-phenyl]methyl]-4-chloranyl-1H-imidazole-5-carboxamide (three-letter code: WHU) (formula: $C_{18}H_{11}BrCl_2FN_5O_2$).
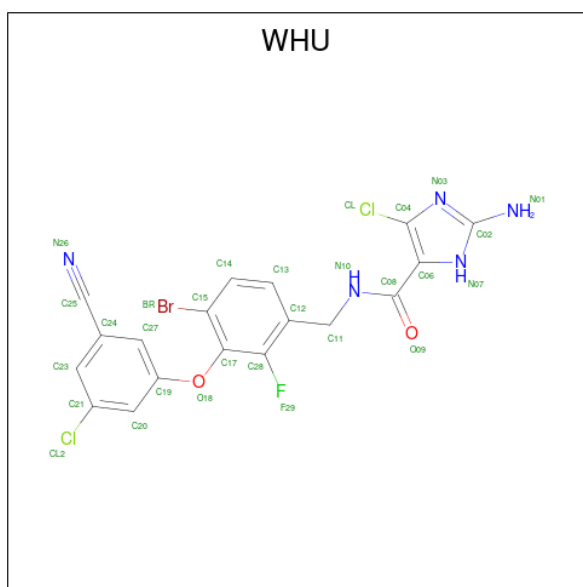
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	Br	C	Cl	F	N	O	0	0
			29	1	18	2	1	5	2		

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	239	Total	O	0	0
			239	239		
6	B	195	Total	O	0	0
			195	195		

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
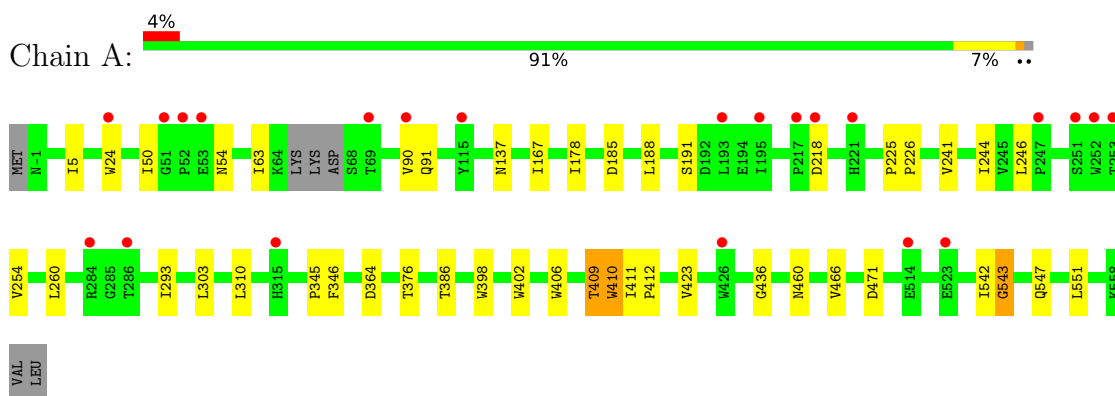
• Molecule 2: P51 RT
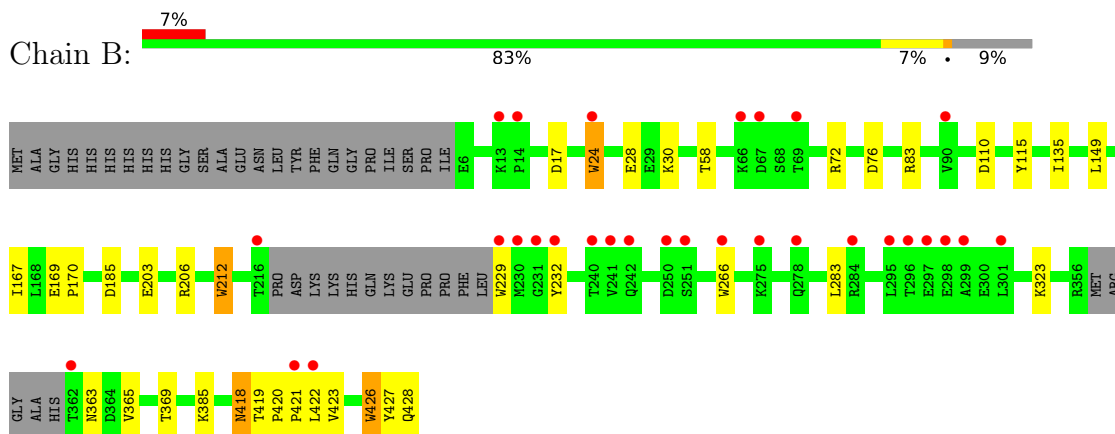
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.58Å 154.51Å 157.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.36 40.52 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.57-2.36) 98.6 (40.52-2.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.45 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.236 0.203 , 0.237	Depositor DCC
R_{free} test set	1783 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å²)	22.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 48.0	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8230	wwPDB-VP
Average B, all atoms (Å²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: TAR, MG, WHU

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	0.66	3/4584 (0.1%)	0.66	0/6242
2	B	0.73	4/3389 (0.1%)	0.71	2/4622 (0.0%)
All	All	0.69	7/7973 (0.1%)	0.68	2/10864 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	TRP	CD2-CE2	6.88	1.49	1.41
2	B	229	TRP	CD2-CE2	6.77	1.49	1.41
1	A	24	TRP	CD2-CE2	5.66	1.48	1.41
1	A	402	TRP	CD2-CE2	5.59	1.48	1.41
1	A	410	TRP	CD2-CE2	5.25	1.47	1.41
2	B	212	TRP	CD2-CE2	5.12	1.47	1.41
2	B	426	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	110	ASP	CB-CG-OD1	6.21	123.88	118.30
2	B	185	ASP	CB-CG-OD1	5.38	123.14	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4463	0	4451	34	0
2	B	3291	0	3239	34	0
3	A	3	0	0	0	0
4	A	10	0	4	2	0
5	A	29	0	11	2	0
6	A	239	0	0	3	0
6	B	195	0	0	4	0
All	All	8230	0	7705	63	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 4.

All (63) 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)
6:A:2160:HOH:O	2:B:418:ASN:HB2	1.86	0.76
1:A:460:ASN:ND2	4:A:1562:TAR:O41	2.18	0.72
1:A:409:THR:HG21	6:A:2137:HOH:O	1.92	0.68
1:A:411:ILE:HG22	1:A:412:PRO:O	1.96	0.66
1:A:398:TRP:CZ2	1:A:411:ILE:HD12	2.31	0.65
2:B:419:THR:C	2:B:421:PRO:CD	2.64	0.65
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.80	0.63
2:B:419:THR:C	2:B:421:PRO:HD2	2.21	0.60
1:A:543:GLY:HA3	2:B:283:LEU:O	2.02	0.60
2:B:418:ASN:O	2:B:418:ASN:ND2	2.25	0.58
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.39	0.57
2:B:72:ARG:NH2	6:B:2047:HOH:O	2.38	0.57
1:A:254:VAL:HG22	1:A:293:ILE:HD11	1.87	0.55
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.41	0.55
2:B:418:ASN:O	2:B:420:PRO:HD3	2.06	0.55
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.37	0.54
1:A:188:LEU:HD13	5:A:1563:WHU:C21	2.37	0.54
1:A:90:VAL:HG23	1:A:91:GLN:N	2.22	0.54
1:A:90:VAL:CG2	1:A:91:GLN:N	2.71	0.53
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.91	0.53
1:A:241:VAL:HG23	1:A:244:ILE:HD11	1.91	0.53
1:A:241:VAL:CG2	1:A:244:ILE:HD11	2.39	0.53
1:A:543:GLY:O	1:A:547:GLN:OE1	2.28	0.52
2:B:58:THR:HG23	2:B:76:ASP:O	2.12	0.50
2:B:24:TRP:HB2	6:B:2011:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:TYR:O	6:B:2076:HOH:O	2.19	0.49
1:A:376:THR:HG23	1:A:386:THR:HG22	1.94	0.48
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.94	0.48
1:A:406:TRP:CZ2	2:B:420:PRO:HB3	2.50	0.47
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.96	0.47
2:B:419:THR:O	2:B:421:PRO:HD2	2.15	0.47
2:B:427:TYR:O	2:B:428:GLN:CB	2.63	0.47
1:A:90:VAL:CG2	1:A:91:GLN:H	2.28	0.47
1:A:90:VAL:HG23	1:A:91:GLN:HG2	1.97	0.47
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.99	0.45
2:B:203:GLU:OE1	2:B:206[B]:ARG:CZ	2.64	0.45
1:A:345:PRO:HA	1:A:346:PHE:HA	1.79	0.45
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.98	0.45
2:B:323:LYS:O	2:B:385:LYS:NZ	2.50	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.37	0.45
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.53	0.44
1:A:188:LEU:HD22	5:A:1563:WHU:C24	2.47	0.44
2:B:421:PRO:HG2	2:B:423:VAL:HG23	1.98	0.44
2:B:17:ASP:O	2:B:83:ARG:HD3	2.19	0.43
1:A:260:LEU:HD21	1:A:303:LEU:HD13	2.01	0.43
1:A:409:THR:HG22	6:A:2163:HOH:O	2.18	0.43
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.54	0.42
1:A:542:ILE:O	1:A:543:GLY:C	2.56	0.42
2:B:266:TRP:CG	2:B:426:TRP:CE3	3.08	0.42
2:B:421:PRO:CG	2:B:423:VAL:HG23	2.49	0.42
2:B:203:GLU:OE1	2:B:206[B]:ARG:NH1	2.53	0.41
2:B:419:THR:C	2:B:421:PRO:HD3	2.41	0.41
2:B:420:PRO:N	2:B:421:PRO:CD	2.83	0.41
1:A:5:ILE:HD12	1:A:167:ILE:HG13	2.03	0.41
2:B:30:LYS:HD3	6:B:2042:HOH:O	2.20	0.41
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.56	0.41
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.09	0.41
2:B:365:VAL:O	2:B:369:THR:HG23	2.20	0.41
2:B:422:LEU:H	2:B:422:LEU:HD12	1.85	0.41
1:A:178:ILE:HD12	1:A:191:SER:HB3	2.03	0.41
1:A:50:ILE:HD12	1:A:54:ASN:HB3	2.04	0.40
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.02	0.40
1:A:436:GLY:CA	4:A:1562:TAR:O3	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/563 (99%)	534 (96%)	19 (3%)	2 (0%)	34	38
2	B	402/447 (90%)	390 (97%)	12 (3%)	0	100	100
All	All	957/1010 (95%)	924 (97%)	31 (3%)	2 (0%)	47	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	GLY
1	A	137	ASN

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	476/503 (95%)	471 (99%)	5 (1%)	73	84
2	B	349/404 (86%)	348 (100%)	1 (0%)	92	96
All	All	825/907 (91%)	819 (99%)	6 (1%)	84	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	185	ASP
1	A	218	ASP
1	A	409	THR

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Mol	Chain	Res	Type
1	A	471	ASP
2	B	418	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	373	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#|Z| > 2$
5	WHU	A	1563	-	29,31,31	1.20	4 (13%)	34,44,44	2.31	8 (23%)
4	TAR	A	1562	-	9,9,9	1.13	0	12,12,12	1.15	1 (8%)

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
5	WHU	A	1563	-	-	1/11/15/15	0/3/3/3
4	TAR	A	1562	-	-	2/12/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1563	WHU	C08-N10	3.07	1.40	1.33
5	A	1563	WHU	C02-N01	2.55	1.39	1.33
5	A	1563	WHU	C17-C15	-2.51	1.35	1.40
5	A	1563	WHU	C02-N07	2.35	1.37	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1563	WHU	BR-C15-C17	-6.63	108.83	118.51
5	A	1563	WHU	BR-C15-C14	6.01	129.50	117.81
5	A	1563	WHU	C12-C11-N10	-5.22	102.02	113.03
5	A	1563	WHU	O18-C17-C15	-3.71	115.27	120.55
5	A	1563	WHU	C23-C24-C25	-2.97	115.58	119.54
5	A	1563	WHU	F29-C28-C12	2.81	120.81	117.85
5	A	1563	WHU	C19-O18-C17	2.34	122.24	118.48
4	A	1562	TAR	O11-C1-C2	2.19	119.19	113.27
5	A	1563	WHU	O18-C17-C28	2.01	125.22	120.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1562	TAR	O1-C1-C2-O2
4	A	1562	TAR	O11-C1-C2-O2
5	A	1563	WHU	C15-C17-O18-C19

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1563	WHU	2	0
4	A	1562	TAR	2	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 WHU A 1563
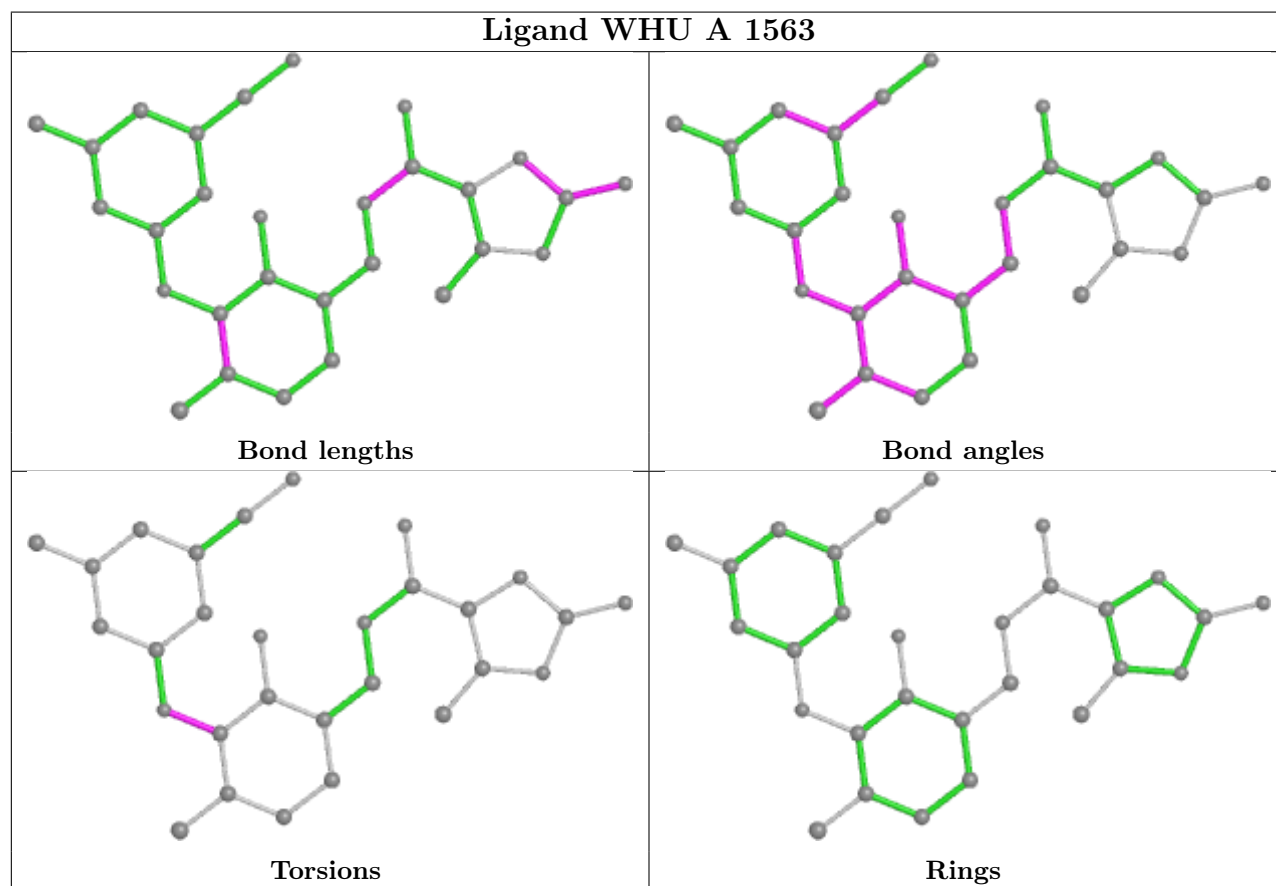
5.7 Other polymers ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	557/563 (98%)	0.19	22 (3%)	39	52	23, 43, 90, 158	0
2	B	406/447 (90%)	0.24	30 (7%)	14	22	19, 38, 73, 88	0
All	All	963/1010 (95%)	0.21	52 (5%)	25	37	19, 41, 80, 158	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	PRO	5.5
2	B	421	PRO	4.1
2	B	67	ASP	3.8
1	A	221	HIS	3.8
2	B	69	THR	3.7
2	B	296	THR	3.6
1	A	284	ARG	3.6
2	B	229	TRP	3.6
2	B	13	LYS	3.6
1	A	286	THR	3.5
2	B	266	TRP	3.4
2	B	14	PRO	3.4
2	B	231	GLY	3.3
2	B	66	LYS	3.3
2	B	362	THR	3.2
2	B	301	LEU	3.2
1	A	195	ILE	3.1
2	B	230	MET	3.0
1	A	251	SER	3.0
2	B	232	TYR	3.0
1	A	69	THR	2.9
2	B	295	LEU	2.9
1	A	252	TRP	2.8
2	B	90	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	298	GLU	2.7
2	B	251	SER	2.7
2	B	240	THR	2.6
1	A	53	GLU	2.5
1	A	218	ASP	2.5
1	A	514	GLU	2.5
1	A	193	LEU	2.4
1	A	426	TRP	2.4
1	A	24	TRP	2.4
2	B	422	LEU	2.4
1	A	523	GLU	2.3
2	B	284	ARG	2.3
2	B	278	GLN	2.3
1	A	217	PRO	2.3
1	A	247	PRO	2.3
2	B	24	TRP	2.2
1	A	51	GLY	2.2
1	A	315	HIS	2.2
2	B	241	VAL	2.2
2	B	242	GLN	2.2
2	B	299	ALA	2.2
2	B	275	LYS	2.1
1	A	115	TYR	2.1
1	A	253	THR	2.1
2	B	216	THR	2.1
2	B	250	ASP	2.0
1	A	90	VAL	2.0
2	B	297	GLU	2.0

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

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

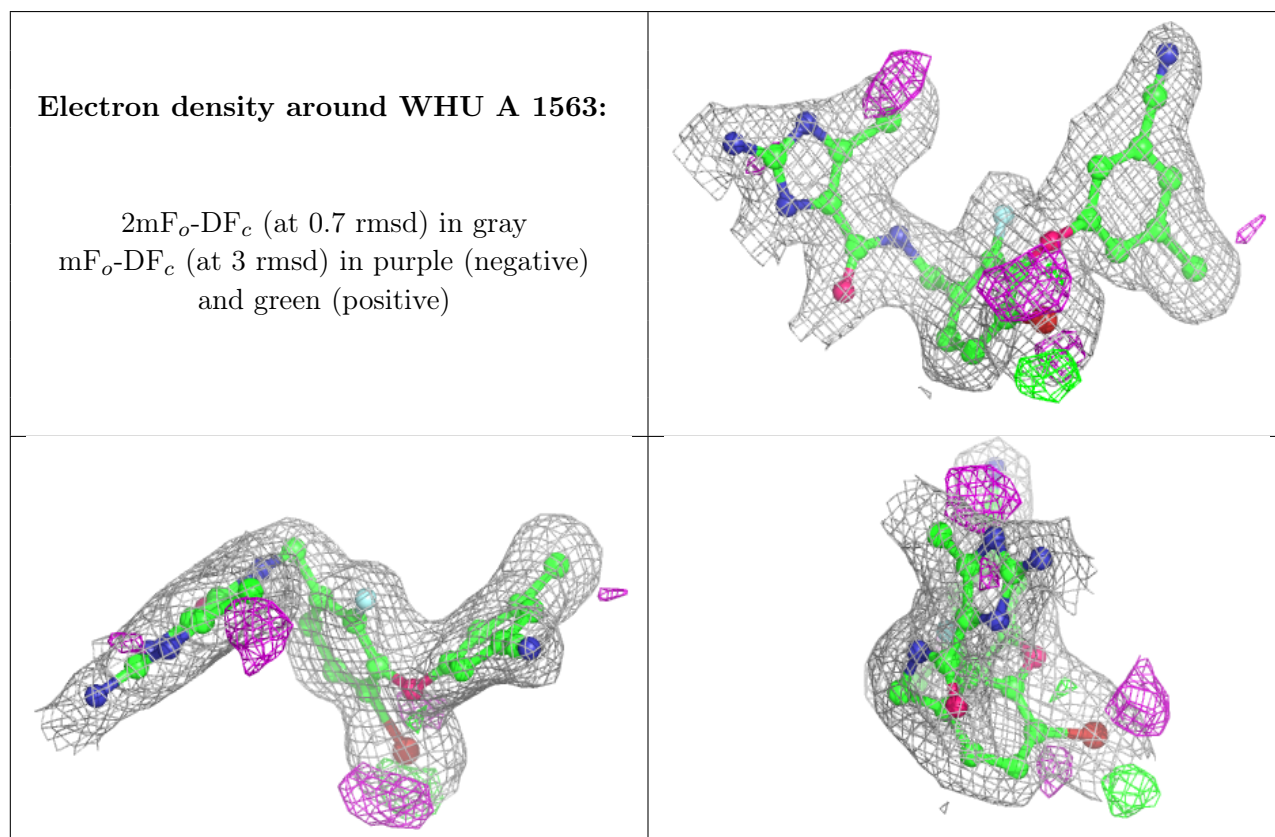## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	MG	A	1561	1/1	0.56	0.56	43,43,43,43	1
4	TAR	A	1562	10/10	0.78	0.22	50,63,75,78	0
3	MG	A	1560	1/1	0.85	0.18	34,34,34,34	1
3	MG	A	1559	1/1	0.94	0.19	55,55,55,55	0
5	WHU	A	1563	29/29	0.96	0.13	29,36,41,51	1

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 WHU A 1563:

$2mF_o$-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 ⓘ

There are no such residues in this entry.