Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:25 am BST

PDB ID	:	2YNI
Title	:	HIV-1 Reverse Transcriptase in complex with inhibitor GSK952
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Deposited on	:	2012-10-15
Resolution	:	2.49 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:

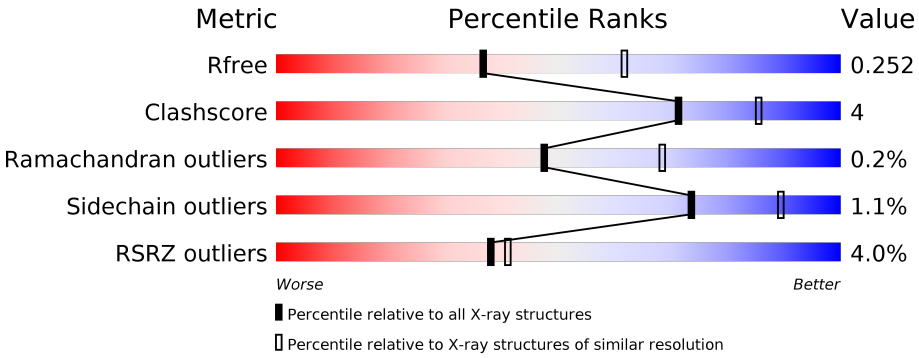
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 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	3% 91% 8%
2	B	447	5% 81% 9% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8268 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	560	Total	C	N	O	S	0	1	0
			4513	2911	753	841	8			

There are 3 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

- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	3	0
			3338	2171	551	608	8			

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
B	-6	GLU	-	expression tag	UNP P04585

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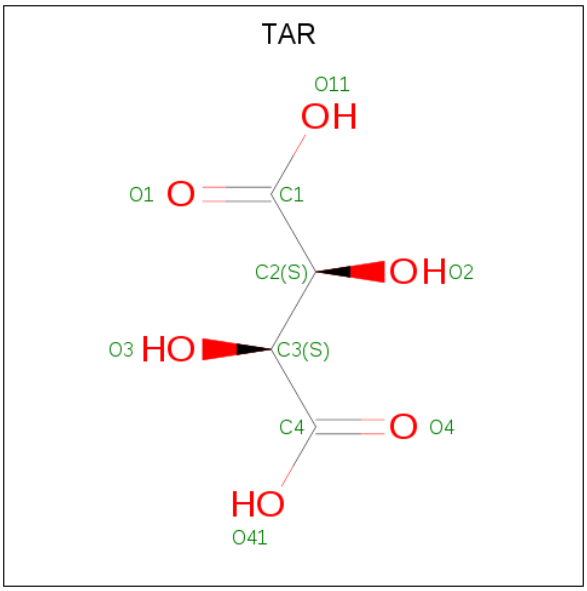
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ASN	-	expression tag	UNP P04585
B	-4	LEU	-	expression tag	UNP P04585
B	-3	TYR	-	expression tag	UNP P04585
B	-2	PHE	-	expression tag	UNP P04585
B	-1	GLN	-	expression tag	UNP P04585
B	0	GLY	-	expression tag	UNP P04585

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

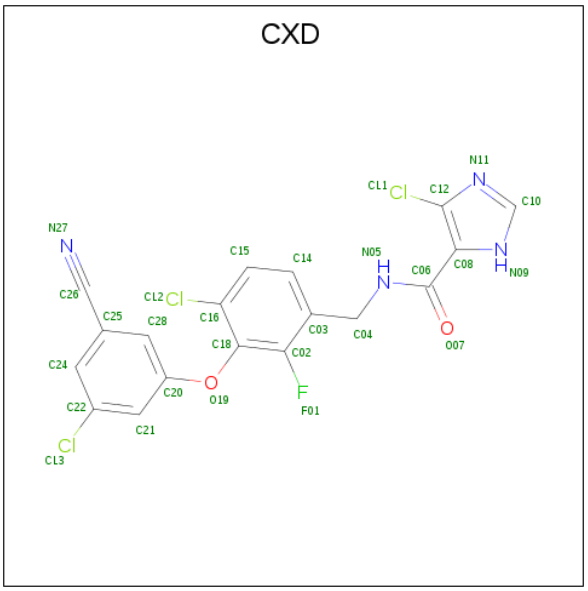
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- 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 C O 10 4 6	0	0

- Molecule 5 is 4-chloranyl-N-[[4-chloranyl-3-(3-chloranyl-5-cyano-phenoxy)-2-fluoranyl-phenyl]methyl]-1H-imidazole-5-carboxamide (three-letter code: CXD) (formula: $C_{18}H_{10}Cl_3FN_4O_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	N	O	0	0
			28	18	3	1	4	2		

- Molecule 6 is water.

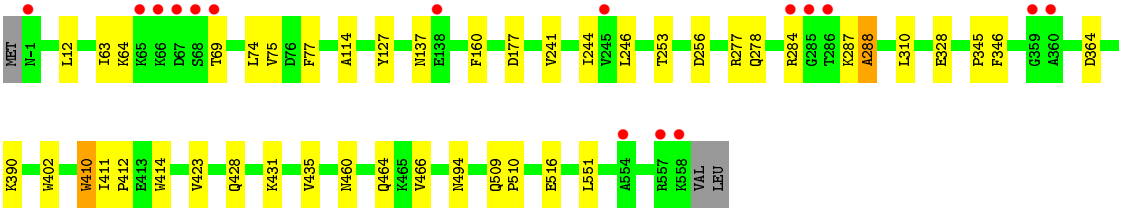
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	0
			220	220		
6	B	158	Total	O	0	0
			158	158		

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 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.

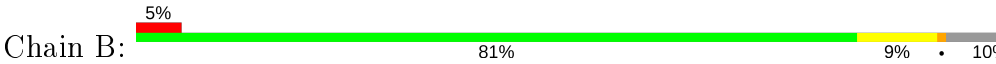
- Molecule 1: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

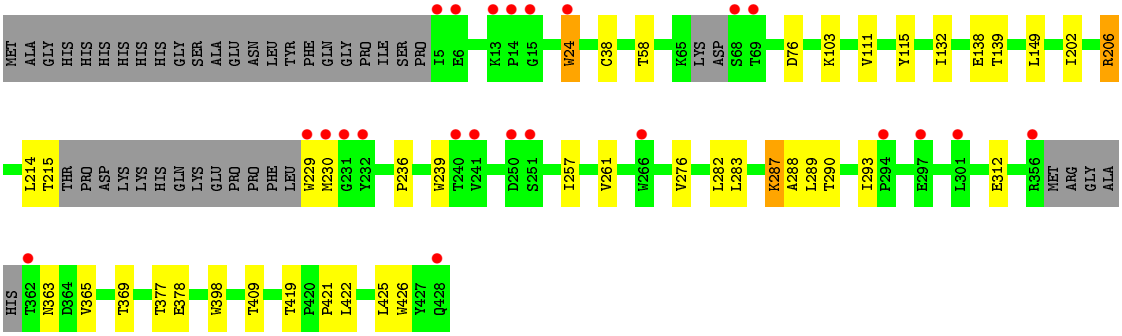
Chain A:



- Molecule 2: P51 RT

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.50Å 154.58Å 156.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 2.49 26.08 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.13-2.49) 100.0 (26.08-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.52 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.254 0.204 , 0.252	Depositor DCC
R_{free} test set	1576 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8268	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: MG, CXD, TAR

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	0.54	3/4630 (0.1%)	0.55	0/6305
2	B	0.58	3/3431 (0.1%)	0.57	0/4669
All	All	0.55	6/8061 (0.1%)	0.56	0/10974

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
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	229	TRP	CD2-CE2	5.49	1.48	1.41
2	B	24	TRP	CD2-CE2	5.35	1.47	1.41
1	A	410	TRP	CD2-CE2	5.20	1.47	1.41
2	B	426	TRP	CD2-CE2	5.09	1.47	1.41
1	A	414	TRP	CD2-CE2	5.03	1.47	1.41
1	A	402	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	419	THR	Peptide

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	4513	0	4483	29	0
2	B	3338	0	3315	33	0
3	A	1	0	0	0	0
4	A	10	0	4	0	0
5	A	28	0	10	0	0
6	A	220	0	0	0	0
6	B	158	0	0	3	0
All	All	8268	0	7812	55	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 (55) 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:422:LEU:HD23	2:B:425:LEU:HD12	1.53	0.90
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.77	0.67
1:A:287:LYS:O	1:A:288:ALA:CB	2.47	0.63
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.34	0.61
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.83	0.61
2:B:287:LYS:HZ2	2:B:293:ILE:HD11	1.71	0.56
2:B:214:LEU:HD23	2:B:215:THR:N	2.20	0.56
2:B:365:VAL:O	2:B:369:THR:HG23	2.05	0.56
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.42	0.55
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.37	0.54
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.21	0.54
2:B:282:LEU:HD23	2:B:293:ILE:HG22	1.90	0.53
2:B:24:TRP:HB2	6:B:2011:HOH:O	2.08	0.53
1:A:244:ILE:HD12	1:A:244:ILE:N	2.25	0.52
2:B:287:LYS:NZ	2:B:293:ILE:HD11	2.26	0.51
1:A:241:VAL:HG23	1:A:244:ILE:HD11	1.94	0.50
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.77	0.50
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.47	0.50
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.47	0.49
1:A:63:ILE:HD11	1:A:74:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:MET:HE2	2:B:377:THR:HG21	1.94	0.49
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.95	0.49
2:B:202:ILE:HG22	2:B:206[B]:ARG:HE	1.78	0.49
1:A:287:LYS:O	1:A:288:ALA:HB3	2.14	0.48
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.95	0.48
2:B:103:LYS:NZ	6:B:2059:HOH:O	2.47	0.47
2:B:111:VAL:HA	2:B:214:LEU:HD21	1.96	0.47
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.54	0.47
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.45	0.47
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.96	0.47
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.50	0.47
1:A:241:VAL:CG2	1:A:244:ILE:HD11	2.45	0.46
1:A:435:VAL:HA	2:B:290:THR:HG21	1.97	0.46
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.98	0.44
2:B:58:THR:HG23	2:B:76:ASP:O	2.17	0.44
1:A:253:THR:HG23	1:A:256:ASP:OD2	2.18	0.44
1:A:177[A]:ASP:N	1:A:177[A]:ASP:OD1	2.47	0.43
1:A:411:ILE:HG22	1:A:412:PRO:O	2.18	0.43
2:B:276:VAL:O	2:B:276:VAL:HG12	2.18	0.43
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.99	0.43
1:A:345:PRO:HA	1:A:346:PHE:HA	1.73	0.43
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.00	0.43
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.53	0.43
1:A:328:GLU:HG2	1:A:390:LYS:HB2	2.01	0.42
1:A:64:LYS:HE3	1:A:69:THR:HA	2.01	0.42
2:B:422:LEU:CD2	2:B:425:LEU:HD12	2.36	0.42
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.50	0.42
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.41
1:A:277:ARG:NH1	1:A:278:GLN:OE1	2.53	0.41
2:B:282:LEU:HB3	2:B:293:ILE:HG21	2.03	0.41
1:A:410:TRP:CE3	2:B:363:ASN:CB	3.04	0.40
2:B:409:THR:HG21	6:B:2066:HOH:O	2.21	0.40
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.56	0.40
2:B:138:GLU:HG2	2:B:139:THR:HG23	2.03	0.40
2:B:282:LEU:HD23	2:B:293:ILE:CG2	2.52	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	559/563 (99%)	536 (96%)	22 (4%)	1 (0%)	47 68
2	B	399/447 (89%)	392 (98%)	6 (2%)	1 (0%)	41 61
All	All	958/1010 (95%)	928 (97%)	28 (3%)	2 (0%)	47 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ALA
2	B	421	PRO

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	486/503 (97%)	480 (99%)	6 (1%)	71 88
2	B	362/404 (90%)	358 (99%)	4 (1%)	73 89
All	All	848/907 (94%)	838 (99%)	10 (1%)	73 88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	284	ARG
1	A	428	GLN
1	A	431	LYS

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Mol	Chain	Res	Type
1	A	464	GLN
1	A	516	GLU
2	B	206[A]	ARG
2	B	206[B]	ARG
2	B	287	LYS
2	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	255	ASN

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 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
4	TAR	A	1560	-	3,9,9	0.47	0	6,12,12	0.85	0
5	CXD	A	1561	-	26,30,30	0.96	2 (7%)	33,42,42	1.59	7 (21%)

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
4	TAR	A	1560	-	-	0/4/12/12	-
5	CXD	A	1561	-	-	0/11/15/15	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1561	CXD	C06-N05	2.58	1.39	1.33
5	A	1561	CXD	C08-C06	-2.25	1.47	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1561	CXD	C03-C04-N05	-5.35	101.74	113.03
5	A	1561	CXD	C20-O19-C18	3.39	123.94	118.48
5	A	1561	CXD	F01-C02-C03	2.79	120.80	117.85
5	A	1561	CXD	C15-C16-CL2	2.58	123.58	118.41
5	A	1561	CXD	C10-N09-C08	2.49	107.74	102.99
5	A	1561	CXD	C18-C16-CL2	-2.12	115.64	118.41
5	A	1561	CXD	F01-C02-C18	-2.09	116.43	119.39

There are no chirality outliers.

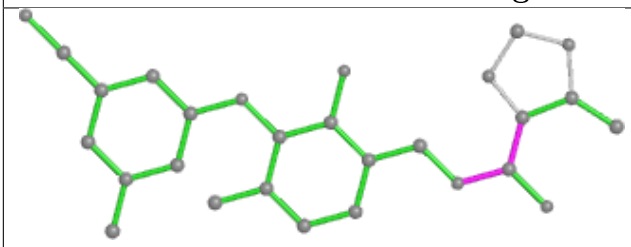
There are no torsion outliers.

There are no ring outliers.

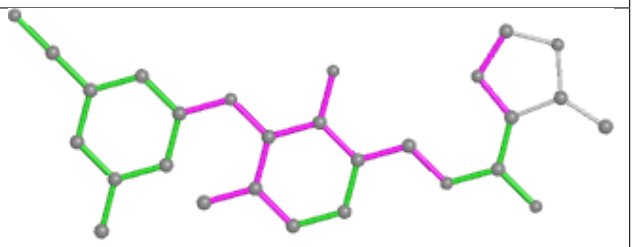
No monomer is involved in short contacts.

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.

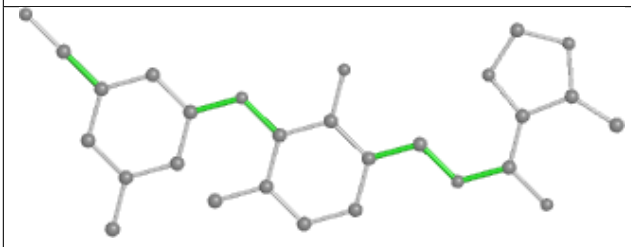
Ligand CXD A 1561



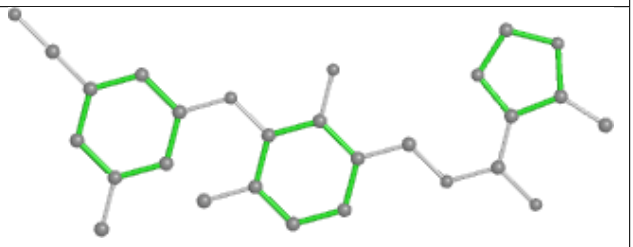
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	560/563 (99%)	-0.10	16 (2%)	51	55	23, 43, 73, 103	0
2	B	404/447 (90%)	-0.01	23 (5%)	23	25	22, 40, 84, 111	0
All	All	964/1010 (95%)	-0.06	39 (4%)	38	41	22, 42, 80, 111	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	4.4
1	A	284	ARG	4.4
2	B	14	PRO	4.2
2	B	69	THR	4.1
1	A	286	THR	4.0
2	B	297	GLU	3.6
2	B	5	ILE	3.6
1	A	285	GLY	3.4
2	B	428	GLN	3.3
2	B	229	TRP	3.1
1	A	67	ASP	2.9
2	B	230	MET	2.9
2	B	232	TYR	2.9
2	B	13	LYS	2.8
2	B	68	SER	2.8
1	A	558	LYS	2.7
2	B	251	SER	2.7
2	B	6	GLU	2.6
1	A	66	LYS	2.6
2	B	15	GLY	2.6
2	B	240	THR	2.6
1	A	-1	ASN	2.6
1	A	68	SER	2.6
1	A	554	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	356	ARG	2.5
1	A	138	GLU	2.5
1	A	557	ARG	2.5
2	B	266	TRP	2.4
1	A	65	LYS	2.4
1	A	245	VAL	2.4
2	B	241	VAL	2.4
2	B	362	THR	2.4
2	B	24	TRP	2.3
2	B	294	PRO	2.3
1	A	360	ALA	2.2
1	A	69	THR	2.2
2	B	250	ASP	2.1
2	B	301	LEU	2.1
1	A	359	GLY	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

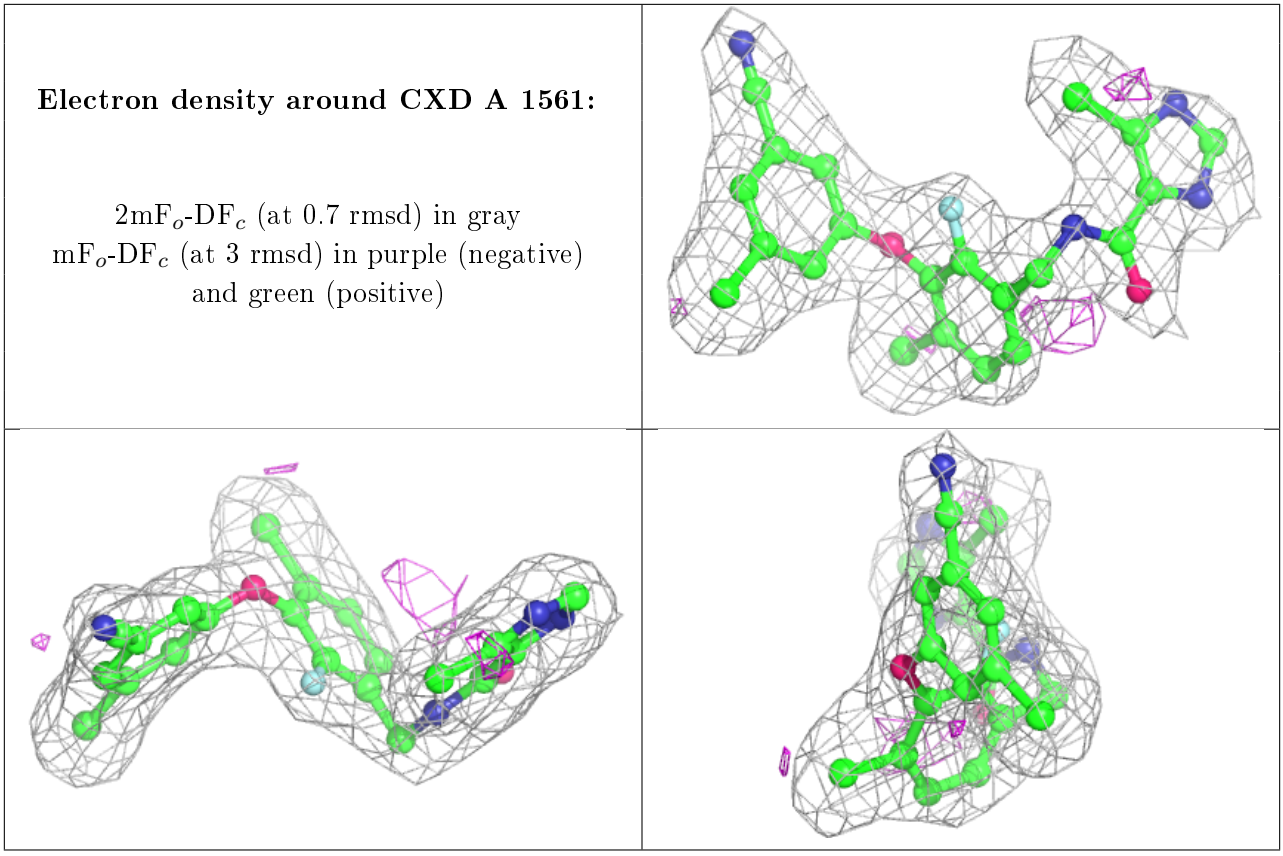
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	1559	1/1	0.86	0.10	55,55,55,55	0
4	TAR	A	1560	10/10	0.86	0.18	62,73,82,82	0
5	CXD	A	1561	28/28	0.96	0.12	30,34,45,50	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 CXD A 1561:

$2mF_o$-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.