



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:38 PM BST

PDB ID : 6DJE
Title : Crystal structure of Tdp1 catalytic domain in complex with Sigma Aldrich compound CDS010292
Authors : Lountos, G.T.; Zhao, X.Z.; Kiselev, E.; Tropea, J.E.; Needle, D.; Burke Jr., T.R.; Pommier, Y.; Waugh, D.S.
Deposited on : 2018-05-25
Resolution : 1.71 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 : 2.13.1
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) : 2.13.1

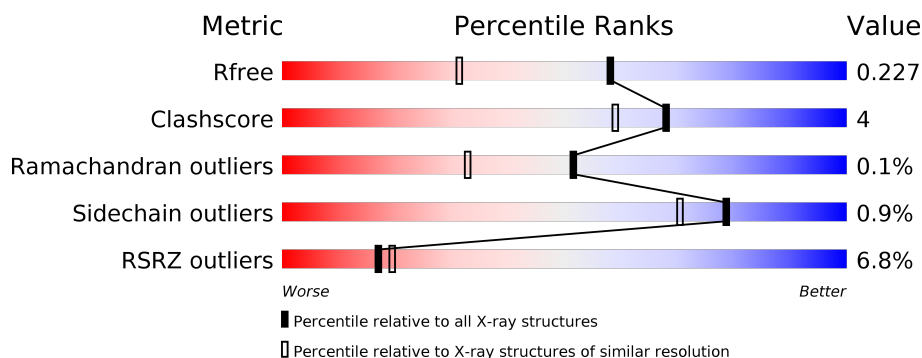
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	461	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

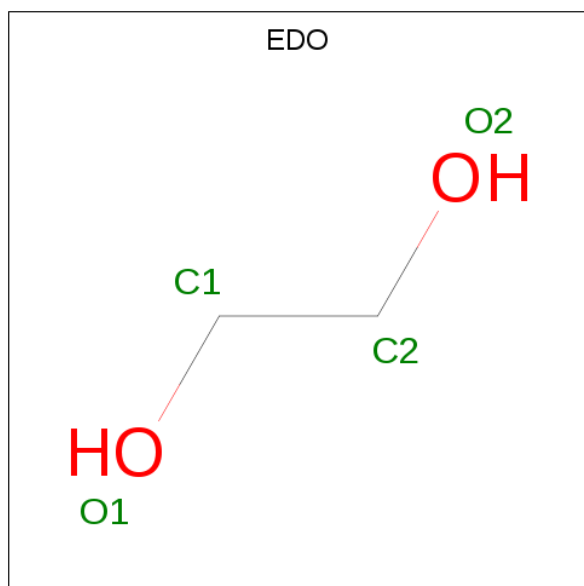
There are 4 unique types of molecules in this entry. The entry contains 7894 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tyrosyl-DNA phosphodiesterase 1.

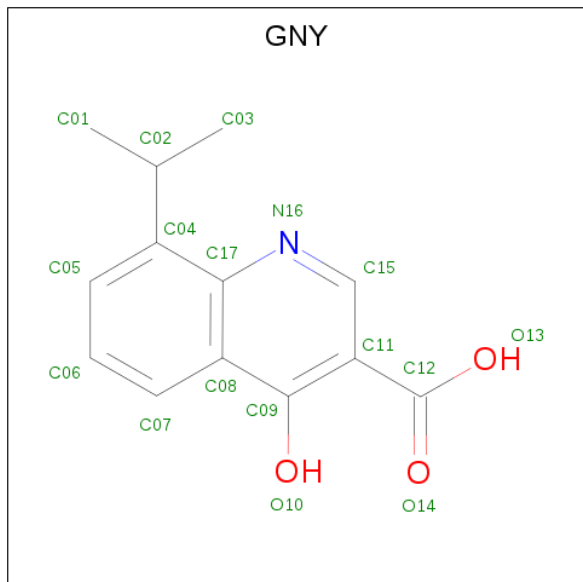
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	16	0
			3609	2335	611	649	14			
1	B	436	Total	C	N	O	S	0	14	0
			3587	2323	603	647	14			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 4-hydroxy-8-(propan-2-yl)quinoline-3-carboxylic acid (three-letter code: GNY) (formula: $C_{13}H_{13}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	13	1	3		
3	B	1	Total	C	N	O	0	0
			17	13	1	3		

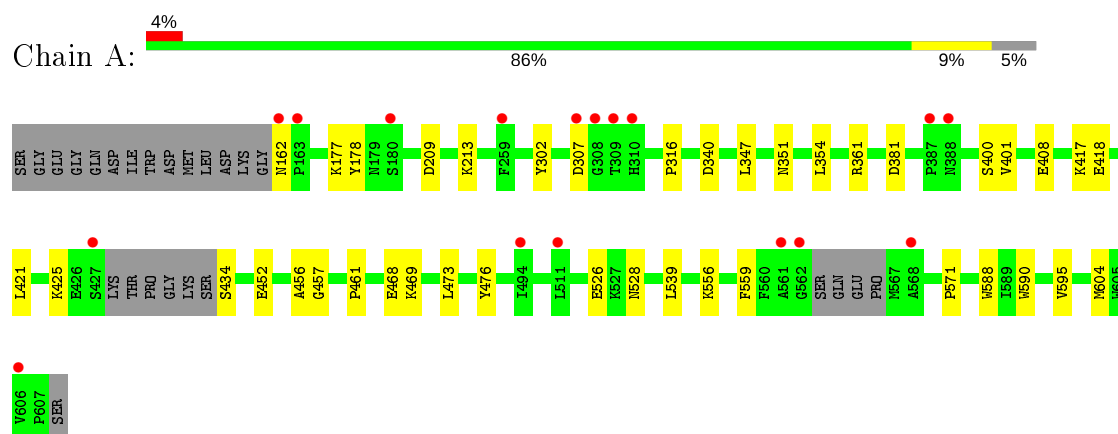
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	391	Total	O	0	0
			391	391		
4	B	257	Total	O	0	0
			257	257		

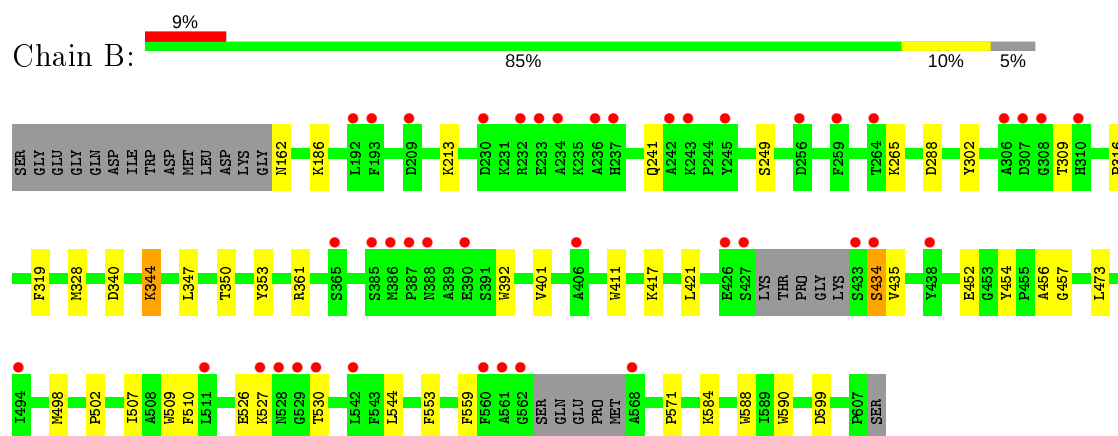
3 Residue-property plots [i](#)

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: Tyrosyl-DNA phosphodiesterase 1



• Molecule 1: Tyrosyl-DNA phosphodiesterase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.06Å 105.37Å 194.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.67 – 1.71 35.67 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.67-1.71) 99.3 (35.67-1.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 1.71Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.191 , 0.227 0.191 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7894	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.37	0/3726	0.54	0/5061
1	B	0.33	0/3703	0.52	0/5032
All	All	0.35	0/7429	0.53	0/10093

There are no bond length outliers.

There are no bond angle outliers.

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	3609	0	3519	26	0
1	B	3587	0	3499	30	0
2	A	12	0	18	0	0
2	B	4	0	6	0	0
3	A	17	0	0	0	0
3	B	17	0	0	1	0
4	A	391	0	0	8	0
4	B	257	0	0	3	0
All	All	7894	0	7042	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)
1:B:498:MET:HE3	1:B:510:PHE:HD1	1.32	0.95
1:B:498:MET:HE3	1:B:510:PHE:CD1	2.19	0.77
1:B:340:ASP:O	1:B:344:LYS:HD2	1.91	0.71
1:A:418:GLU:OE1	4:A:801:HOH:O	2.12	0.67
1:B:241:GLN:NE2	4:B:803:HOH:O	2.29	0.65
1:A:556:LYS:NZ	4:A:810:HOH:O	2.30	0.64
1:B:498:MET:HE2	1:B:507:ILE:HG21	1.80	0.63
1:B:328[B]:MET:SD	4:B:929:HOH:O	2.56	0.61
1:A:351[B]:ASN:OD1	4:A:802:HOH:O	2.16	0.60
1:A:209[B]:ASP:OD1	1:A:213:LYS:NZ	2.30	0.59
1:A:162:ASN:N	4:A:812:HOH:O	2.36	0.58
1:B:498:MET:CE	1:B:507:ILE:HG21	2.35	0.56
1:A:340:ASP:OD2	4:A:803:HOH:O	2.18	0.56
1:B:452:GLU:HB2	1:B:456:ALA:HB2	1.87	0.56
1:B:527:LYS:O	1:B:530:THR:HG22	2.06	0.55
1:B:186:LYS:NZ	1:B:213:LYS:O	2.42	0.53
1:B:584:LYS:HD3	1:B:584:LYS:N	2.22	0.53
1:A:468:GLU:OE2	1:A:469:LYS:NZ	2.41	0.52
1:B:457:GLY:HA3	1:B:588:TRP:CZ2	2.46	0.51
1:A:400:SER:HB3	1:A:461:PRO:HD2	1.94	0.49
1:B:421[A]:LEU:HD21	1:B:435:VAL:HG11	1.94	0.48
1:A:361[B]:ARG:NH1	1:A:526:GLU:OE1	2.46	0.48
1:A:559:PHE:CE1	1:A:571:PRO:HB2	2.48	0.48
1:A:401:VAL:HG11	1:A:473:LEU:HD21	1.96	0.48
1:B:434:SER:OG	1:B:434:SER:O	2.32	0.47
1:B:417:LYS:HE2	1:B:421[A]:LEU:HD11	1.97	0.47
1:B:509:TRP:HB3	1:B:544:LEU:HD23	1.96	0.47
1:B:265:LYS:HZ1	3:B:702:GNV:C12	2.27	0.47
1:B:507:ILE:HG13	1:B:553:PHE:HB2	1.96	0.47
1:B:353:TYR:CE2	1:B:544:LEU:HD12	2.50	0.46
1:A:457:GLY:HA3	1:A:588:TRP:CZ2	2.50	0.46
1:A:408:GLU:OE1	1:A:476:TYR:OH	2.28	0.46
1:A:452:GLU:HB2	1:A:456:ALA:HB2	1.96	0.46
1:B:309:THR:OG1	4:B:801:HOH:O	2.21	0.45
1:A:177:LYS:HE3	1:A:178:TYR:CZ	2.52	0.44
1:A:354:LEU:HD11	1:A:539:LEU:HD11	2.00	0.44
1:B:559:PHE:CE1	1:B:571:PRO:HB2	2.52	0.44
1:B:457:GLY:HA3	1:B:588:TRP:CE2	2.53	0.43
1:A:302:TYR:CD1	1:A:347:LEU:HA	2.54	0.43
1:B:361[B]:ARG:NH1	1:B:526:GLU:OE1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ASN:OD1	4:A:804:HOH:O	2.22	0.42
1:A:316:PRO:HA	1:B:316:PRO:HA	2.00	0.42
1:B:421[A]:LEU:HA	1:B:421[A]:LEU:HD23	1.85	0.42
1:B:392:TRP:CD1	1:B:502:PRO:HD3	2.54	0.42
1:B:302:TYR:CD1	1:B:347:LEU:HA	2.55	0.42
1:B:319:PHE:CG	1:B:350:THR:HG21	2.54	0.42
1:B:454:TYR:CD2	1:B:599:ASP:HB3	2.55	0.42
1:A:434:SER:N	4:A:826:HOH:O	2.53	0.41
1:A:307:ASP:O	4:A:805:HOH:O	2.22	0.41
1:A:417[B]:LYS:O	1:A:421:LEU:HG	2.20	0.41
1:A:595:VAL:HA	1:A:604:MET:HE2	2.03	0.41
1:B:401:VAL:HG11	1:B:473:LEU:HD21	2.02	0.41
1:A:381:ASP:OD1	1:A:425:LYS:NZ	2.54	0.40
1:A:468:GLU:HG3	1:A:469:LYS:HD3	2.02	0.40
1:A:417[A]:LYS:O	1:A:421:LEU:HG	2.22	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	446/461 (97%)	435 (98%)	11 (2%)	0	100	100
1	B	444/461 (96%)	435 (98%)	8 (2%)	1 (0%)	47	30
All	All	890/922 (96%)	870 (98%)	19 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411	TRP

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	393/400 (98%)	392 (100%)	1 (0%)	92	89
1	B	391/400 (98%)	385 (98%)	6 (2%)	65	51
All	All	784/800 (98%)	777 (99%)	7 (1%)	78	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	590	TRP
1	B	162	ASN
1	B	249	SER
1	B	288	ASP
1	B	344	LYS
1	B	434	SER
1	B	590	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

6 ligands are modelled in this entry.

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$
2	EDO	B	701	-	3,3,3	0.53	0	2,2,2	0.36	0
3	GNY	B	702	-	16,18,18	2.19	2 (12%)	19,26,26	1.58	2 (10%)
2	EDO	A	702	-	3,3,3	0.54	0	2,2,2	0.27	0
2	EDO	A	701	-	3,3,3	0.40	0	2,2,2	0.44	0
3	GNY	A	704	-	16,18,18	2.07	2 (12%)	19,26,26	1.47	3 (15%)
2	EDO	A	703	-	3,3,3	0.50	0	2,2,2	0.24	0

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
2	EDO	B	701	-	-	0/1/1/1	-
3	GNY	B	702	-	-	0/4/8/8	0/2/2/2
2	EDO	A	702	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
3	GNY	A	704	-	-	0/4/8/8	0/2/2/2
2	EDO	A	703	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	GNY	C11-C12	6.51	1.53	1.47
3	A	704	GNY	C11-C12	5.95	1.53	1.47
3	B	702	GNY	O10-C09	-4.90	1.19	1.35
3	A	704	GNY	O10-C09	-4.63	1.20	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	702	GNV	C15-N16-C17	5.32	122.09	116.78
3	A	704	GNV	C15-N16-C17	4.72	121.49	116.78
3	B	702	GNV	C11-C15-N16	-2.36	120.87	124.52
3	A	704	GNV	C11-C15-N16	-2.28	121.00	124.52
3	A	704	GNV	C11-C09-C08	-2.19	117.72	120.77

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	B	702	GNV	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/461 (94%)	0.21	17 (3%) 39 44	12, 22, 43, 73	0
1	B	436/461 (94%)	0.56	42 (9%) 8 9	16, 29, 56, 80	0
All	All	872/922 (94%)	0.39	59 (6%) 17 19	12, 26, 50, 80	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	GLY	6.4
1	B	236	ALA	5.7
1	B	561	ALA	5.4
1	A	562	GLY	5.2
1	B	307	ASP	5.1
1	B	365	SER	5.0
1	B	560	PHE	4.4
1	B	209[A]	ASP	4.2
1	B	528	ASN	4.2
1	B	387	PRO	3.9
1	B	306	ALA	3.6
1	B	427	SER	3.6
1	B	233	GLU	3.5
1	A	308	GLY	3.3
1	A	387	PRO	3.3
1	B	308	GLY	3.2
1	B	245	TYR	3.1
1	A	307	ASP	3.1
1	B	259	PHE	3.1
1	B	310	HIS	3.1
1	A	427	SER	3.0
1	B	234	ALA	3.0
1	B	568	ALA	3.0
1	B	530	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	406	ALA	2.9
1	A	606	VAL	2.8
1	A	494	ILE	2.7
1	B	390	GLU	2.7
1	B	433	SER	2.7
1	B	527	LYS	2.6
1	B	237	HIS	2.6
1	B	388	ASN	2.6
1	B	242	ALA	2.4
1	A	180	SER	2.4
1	A	511	LEU	2.4
1	B	264	THR	2.4
1	B	511	LEU	2.4
1	A	259	PHE	2.3
1	B	386	MET	2.3
1	A	568	ALA	2.3
1	B	230	ASP	2.3
1	A	310	HIS	2.3
1	A	388	ASN	2.3
1	B	529	GLY	2.3
1	B	193	PHE	2.3
1	B	243	LYS	2.3
1	B	434	SER	2.2
1	B	494	ILE	2.2
1	B	426	GLU	2.2
1	A	163	PRO	2.2
1	B	438	TYR	2.1
1	A	561	ALA	2.1
1	B	232	ARG	2.1
1	A	309	THR	2.1
1	B	542	LEU	2.1
1	B	385	SER	2.1
1	B	192	LEU	2.0
1	A	162	ASN	2.0
1	B	256	ASP	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 [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(\AA^2)	Q<0.9
3	GNY	A	704	17/17	0.83	0.15	24,30,41,42	17
3	GNY	B	702	17/17	0.86	0.16	31,34,40,47	17
2	EDO	A	701	4/4	0.90	0.15	34,37,38,39	0
2	EDO	A	703	4/4	0.91	0.23	32,36,39,41	0
2	EDO	B	701	4/4	0.94	0.13	22,23,28,29	0
2	EDO	A	702	4/4	0.96	0.11	18,19,21,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.