



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:30 PM UTC

PDB ID : 6DJF / pdb_00006djf
Title : Crystal structure of Tdp1 catalytic domain in complex with compound XZ502
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 : 1.67 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

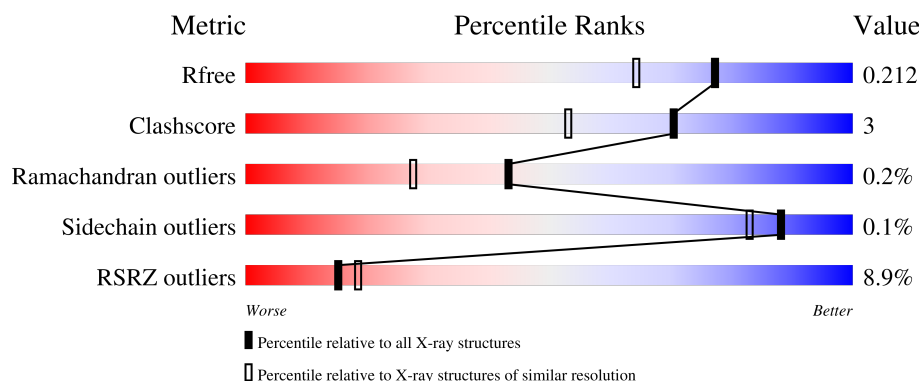
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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 $\leq 5\%$. 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	5% 88% 7% 5%
1	B	461	12% 86% 9% 5%

2 Entry composition [i](#)

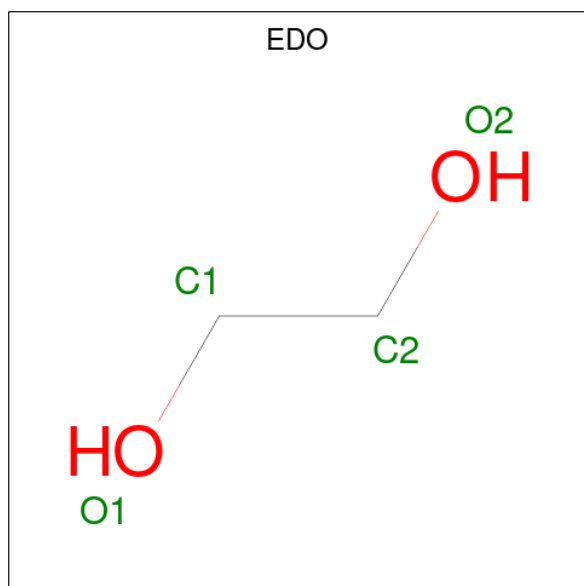
There are 4 unique types of molecules in this entry. The entry contains 7901 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

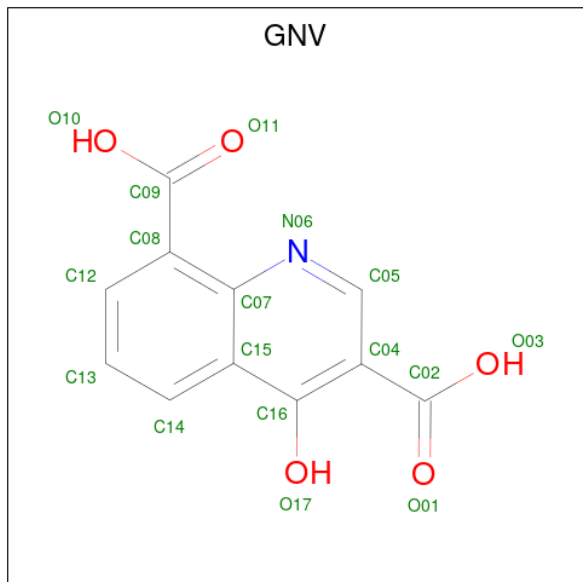
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	16	0
			3616	2341	609	652	14			
1	B	438	Total	C	N	O	S	0	16	0
			3616	2341	609	652	14			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is 4-hydroxyquinoline-3,8-dicarboxylic acid (CCD ID: GNV) (formula: $C_{11}H_7NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	11	1	5		
3	B	1	Total	C	N	O	0	0
			17	11	1	5		

- Molecule 4 is water.

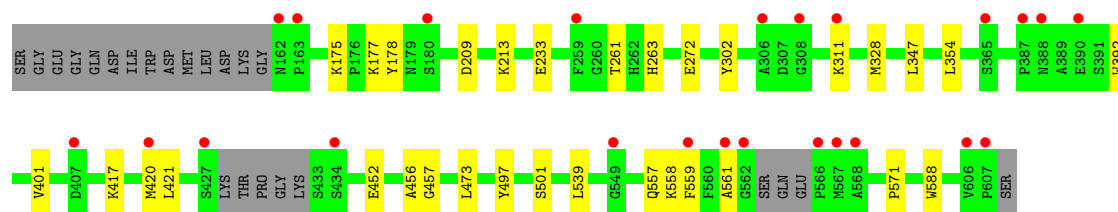
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	363	Total	O	0	0
			363	363		
4	B	256	Total	O	0	0
			256	256		

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.

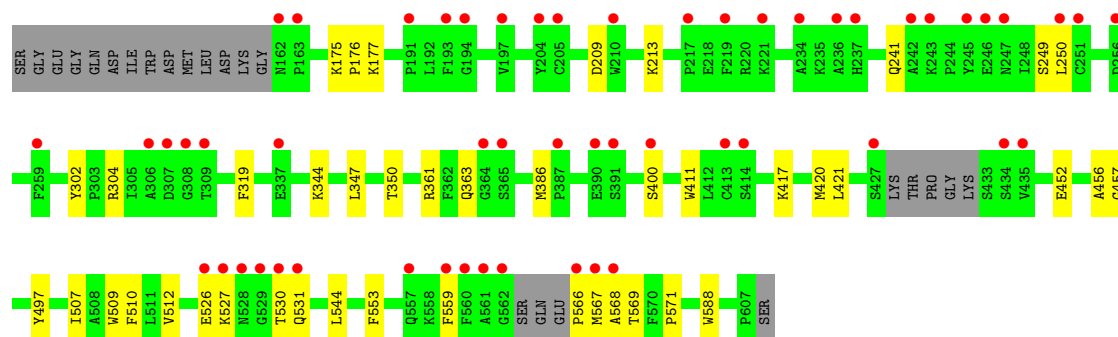
• Molecule 1: Tyrosyl-DNA phosphodiesterase 1

Chain A: 



• Molecule 1: Tyrosyl-DNA phosphodiesterase 1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.16Å 105.31Å 193.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.70 – 1.67 35.70 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.70-1.67) 99.5 (35.70-1.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.36 (at 1.67Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.188 , 0.212 0.189 , 0.212	Depositor DCC
R_{free} test set	2000 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7901	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: GNV, 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	0.28	0/3734	0.50	0/5073
1	B	0.24	0/3733	0.47	0/5072
All	All	0.26	0/7467	0.48	0/10145

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	3616	0	3529	23	0
1	B	3616	0	3531	26	0
2	A	4	0	6	0	0
2	B	12	0	18	0	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
4	A	363	0	0	5	0
4	B	256	0	0	1	0
All	All	7901	0	7084	49	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 3.

All (49) 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:328[B]:MET:SD	4:A:1087:HOH:O	2.43	0.76
1:A:420:MET:HE1	1:A:497:TYR:CD2	2.24	0.72
1:B:304:ARG:NH2	1:B:344:LYS:HD3	2.11	0.65
1:A:272:GLU:OE2	4:A:801:HOH:O	2.14	0.65
1:B:175:LYS:HD3	1:B:176:PRO:HD2	1.80	0.61
1:B:175:LYS:HD2	1:B:177:LYS:H	1.68	0.59
1:B:363:GLN:HG3	1:B:531:GLN:HG3	1.89	0.54
1:A:557:GLN:NE2	4:A:813:HOH:O	2.40	0.54
1:A:175:LYS:NZ	4:A:809:HOH:O	2.37	0.53
1:A:417:LYS:O	1:A:421[A]:LEU:HG	2.09	0.52
1:B:241:GLN:NE2	4:B:808:HOH:O	2.40	0.52
1:A:311:LYS:NZ	4:A:817:HOH:O	2.43	0.51
1:B:566:PRO:O	1:B:569:THR:HG23	2.11	0.51
1:B:509:TRP:HB3	1:B:544:LEU:HD23	1.91	0.51
1:A:558:LYS:HB2	1:A:561:ALA:HB2	1.93	0.50
1:B:420:MET:HE1	1:B:497:TYR:HB3	1.94	0.49
1:A:457:GLY:HA3	1:A:588:TRP:CZ2	2.48	0.49
1:B:417:LYS:O	1:B:421[A]:LEU:HG	2.12	0.48
1:A:420:MET:HE1	1:A:497:TYR:CG	2.48	0.48
1:A:559:PHE:CE2	1:A:571:PRO:HB2	2.48	0.48
1:B:420:MET:HE1	1:B:497:TYR:CB	2.44	0.48
1:B:304:ARG:HH22	1:B:344:LYS:HD3	1.77	0.48
1:B:302:TYR:CD1	1:B:347:LEU:HA	2.49	0.47
1:B:559:PHE:CE2	1:B:571:PRO:HB2	2.50	0.47
1:B:457:GLY:HA3	1:B:588:TRP:CZ2	2.51	0.46
1:B:361[B]:ARG:NH1	1:B:526:GLU:OE1	2.49	0.46
1:A:452:GLU:HB2	1:A:456:ALA:HB2	1.98	0.45
1:B:249:SER:C	1:B:250:LEU:HD12	2.42	0.44
1:B:363:GLN:HG3	1:B:531:GLN:CG	2.47	0.44
1:A:311:LYS:HB2	1:A:311:LYS:HE2	1.77	0.44
1:A:233:GLU:H	1:A:233:GLU:CD	2.25	0.44
1:B:527:LYS:HB2	1:B:530:THR:HG22	1.98	0.44
1:A:209[B]:ASP:OD1	1:A:213:LYS:NZ	2.42	0.43
1:B:452:GLU:HB2	1:B:456:ALA:HB2	2.00	0.43
1:B:507:ILE:HG13	1:B:553:PHE:HB2	2.01	0.43
1:B:510:PHE:HE1	1:B:512[B]:VAL:HG22	1.84	0.42
1:A:457:GLY:HA3	1:A:588:TRP:CE2	2.54	0.42
1:A:261:THR:OG1	1:A:263:HIS:CE1	2.72	0.42
1:A:401:VAL:HG11	1:A:473:LEU:HD21	2.01	0.42
1:B:209[B]:ASP:OD1	1:B:213:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:MET:HE1	1:B:497:TYR:CG	2.54	0.41
1:B:566:PRO:O	1:B:568:ALA:N	2.53	0.41
1:B:319:PHE:CG	1:B:350:THR:HG21	2.56	0.41
1:A:177:LYS:HE3	1:A:178:TYR:CZ	2.56	0.41
1:A:354:LEU:HD11	1:A:539:LEU:HD11	2.02	0.41
1:A:558:LYS:HB2	1:A:561:ALA:CB	2.51	0.41
1:B:386:MET:HE3	1:B:386:MET:HB3	1.90	0.41
1:A:302:TYR:CD1	1:A:347:LEU:HA	2.56	0.40
1:A:392:TRP:CD2	1:A:501:SER:HA	2.57	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	448/461 (97%)	437 (98%)	11 (2%)	0	100	100
1	B	448/461 (97%)	438 (98%)	8 (2%)	2 (0%)	30	13
All	All	896/922 (97%)	875 (98%)	19 (2%)	2 (0%)	43	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	411	TRP
1	B	567	MET

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	395/400 (99%)	395 (100%)	0	100	100
1	B	395/400 (99%)	393 (100%)	2 (0%)	81	72
All	All	790/800 (99%)	788 (100%)	2 (0%)	88	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	400[A]	SER
1	B	400[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	557	GLN
1	B	237	HIS
1	B	531	GLN
1	B	557	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 oligosaccharides 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	703	-	3,3,3	0.45	0	2,2,2	0.25	0
2	EDO	B	702	-	3,3,3	0.43	0	2,2,2	0.39	0
3	GNV	B	704	-	18,18,18	1.64	1 (5%)	23,26,26	1.44	4 (17%)
3	GNV	A	702	-	18,18,18	1.64	1 (5%)	23,26,26	1.42	3 (13%)
2	EDO	B	701	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	A	701	-	3,3,3	0.50	0	2,2,2	0.37	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	703	-	-	1/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
3	GNV	B	704	-	-	6/8/8/8	0/2/2/2
3	GNV	A	702	-	-	0/8/8/8	0/2/2/2
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GNV	O17-C16	-4.99	1.19	1.35
3	B	704	GNV	O17-C16	-4.95	1.19	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GNV	C05-N06-C07	2.76	120.28	116.86
3	B	704	GNV	C05-N06-C07	2.52	119.98	116.86
3	B	704	GNV	C16-C04-C02	2.42	122.42	119.94
3	B	704	GNV	C12-C08-C09	2.23	120.07	116.75
3	A	702	GNV	C04-C05-N06	-2.23	122.30	125.20
3	B	704	GNV	C04-C16-C15	-2.14	117.88	120.69
3	A	702	GNV	O10-C09-C08	2.06	119.83	114.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	704	GNV	C07-C08-C09-O10
3	B	704	GNV	C12-C08-C09-O10
3	B	704	GNV	C12-C08-C09-O11
3	B	704	GNV	O01-C02-C04-C05
3	B	704	GNV	O03-C02-C04-C05
3	B	704	GNV	C07-C08-C09-O11
2	B	703	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	438/461 (95%)	0.26	24 (5%)	30 39	7, 21, 44, 73	16 (3%)
1	B	438/461 (95%)	0.81	54 (12%)	8 11	6, 27, 56, 82	16 (3%)
All	All	876/922 (95%)	0.53	78 (8%)	15 18	6, 24, 50, 82	32 (3%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ALA	7.6
1	B	566	PRO	6.9
1	B	568	ALA	6.2
1	B	567	MET	5.3
1	A	566	PRO	5.0
1	A	163	PRO	4.5
1	A	162	ASN	4.4
1	B	365	SER	4.1
1	B	308	GLY	4.0
1	A	568	ALA	4.0
1	A	306	ALA	4.0
1	A	365	SER	3.8
1	A	427	SER	3.8
1	B	530	THR	3.8
1	B	562	GLY	3.5
1	B	217	PRO	3.5
1	B	387	PRO	3.4
1	B	529	GLY	3.3
1	B	414	SER	3.3
1	B	307	ASP	3.1
1	B	205[A]	CYS	3.1
1	B	242	ALA	3.1
1	A	387	PRO	3.0
1	B	561	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	259	PHE	3.0
1	B	309	THR	3.0
1	B	559	PHE	3.0
1	B	528	ASN	3.0
1	B	427	SER	2.9
1	A	390	GLU	2.9
1	B	251	CYS	2.9
1	B	527	LYS	2.9
1	B	434	SER	2.8
1	B	390	GLU	2.8
1	B	364	GLY	2.8
1	B	391	SER	2.8
1	A	308	GLY	2.8
1	B	247	ASN	2.7
1	B	236	ALA	2.7
1	B	560	PHE	2.7
1	A	388	ASN	2.7
1	B	259	PHE	2.7
1	A	180	SER	2.7
1	B	162	ASN	2.6
1	B	163	PRO	2.6
1	B	413	CYS	2.6
1	B	197	VAL	2.6
1	B	219	PHE	2.5
1	A	606	VAL	2.5
1	B	557	GLN	2.5
1	A	567	MET	2.5
1	B	245	TYR	2.5
1	A	562	GLY	2.5
1	B	204	TYR	2.4
1	B	246	GLU	2.4
1	B	526	GLU	2.4
1	B	191[A]	PRO	2.4
1	B	234	ALA	2.3
1	A	561	ALA	2.3
1	B	237	HIS	2.3
1	A	607	PRO	2.3
1	A	434	SER	2.3
1	B	210	TRP	2.2
1	B	250	LEU	2.2
1	B	193	PHE	2.2
1	B	435	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	311	LYS	2.2
1	B	400[A]	SER	2.2
1	A	549	GLY	2.2
1	B	531	GLN	2.2
1	B	337	GLU	2.2
1	A	420	MET	2.1
1	A	407	ASP	2.1
1	B	243	LYS	2.1
1	A	559	PHE	2.1
1	B	194	GLY	2.0
1	B	256	ASP	2.0
1	B	221	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 oligosaccharides 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
2	EDO	B	702	4/4	0.83	0.18	31,43,43,48	0
3	GNV	B	704	17/17	0.86	0.12	28,36,48,64	0
3	GNV	A	702	17/17	0.89	0.10	28,36,50,50	0
2	EDO	B	703	4/4	0.91	0.15	34,34,42,43	0
2	EDO	A	701	4/4	0.96	0.09	18,18,19,21	0
2	EDO	B	701	4/4	0.97	0.10	20,21,24,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.