



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:36 AM UTC

PDB ID : 5INN / pdb_00005inn
Title : Mouse Tdp2 D358N protein, apo state with increased disorder amongst variable DNA-binding grasp conformations
Authors : Schellenberg, M.J.; Appel, C.D.; Williams, R.S.
Deposited on : 2016-03-07
Resolution : 2.80 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

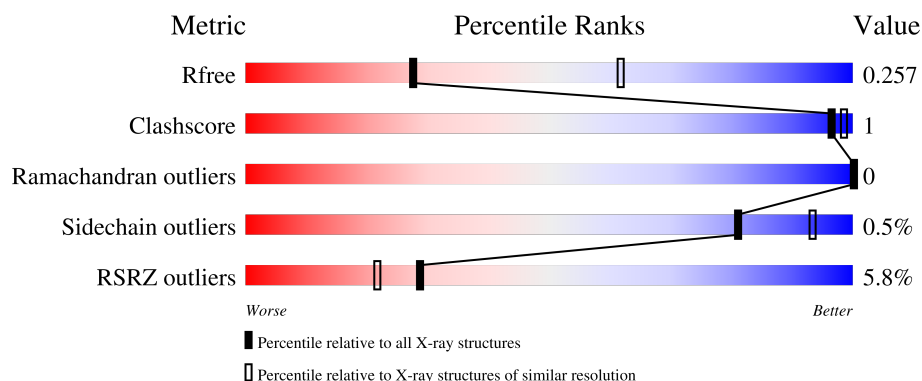
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	256	4% 92% 5%
1	B	256	5% 89% 9%
1	C	256	7% 85% 11%
1	D	256	7% 92%
1	E	256	4% 89% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9587 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1924	1225	333	351	15			
1	B	233	Total	C	N	O	S	0	1	0
			1861	1192	321	334	14			
1	C	229	Total	C	N	O	S	0	0	0
			1824	1169	316	326	13			
1	D	245	Total	C	N	O	S	0	1	0
			1952	1245	336	357	14			
1	E	233	Total	C	N	O	S	0	0	0
			1850	1182	320	334	14			

There are 20 discrepancies between the modelled and reference sequences:

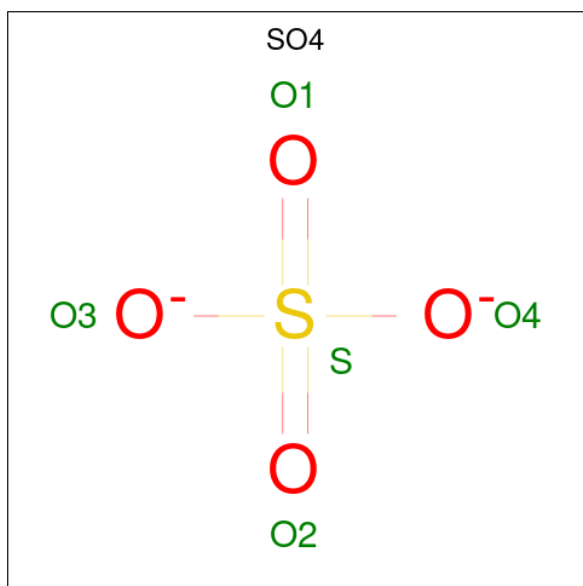
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	-	expression tag	UNP Q9JJX7
A	116	LYS	-	expression tag	UNP Q9JJX7
A	117	GLY	-	expression tag	UNP Q9JJX7
A	358	ASN	ASP	engineered mutation	UNP Q9JJX7
B	115	SER	-	expression tag	UNP Q9JJX7
B	116	LYS	-	expression tag	UNP Q9JJX7
B	117	GLY	-	expression tag	UNP Q9JJX7
B	358	ASN	ASP	engineered mutation	UNP Q9JJX7
C	115	SER	-	expression tag	UNP Q9JJX7
C	116	LYS	-	expression tag	UNP Q9JJX7
C	117	GLY	-	expression tag	UNP Q9JJX7
C	358	ASN	ASP	engineered mutation	UNP Q9JJX7
D	115	SER	-	expression tag	UNP Q9JJX7
D	116	LYS	-	expression tag	UNP Q9JJX7
D	117	GLY	-	expression tag	UNP Q9JJX7
D	358	ASN	ASP	engineered mutation	UNP Q9JJX7
E	115	SER	-	expression tag	UNP Q9JJX7
E	116	LYS	-	expression tag	UNP Q9JJX7
E	117	GLY	-	expression tag	UNP Q9JJX7

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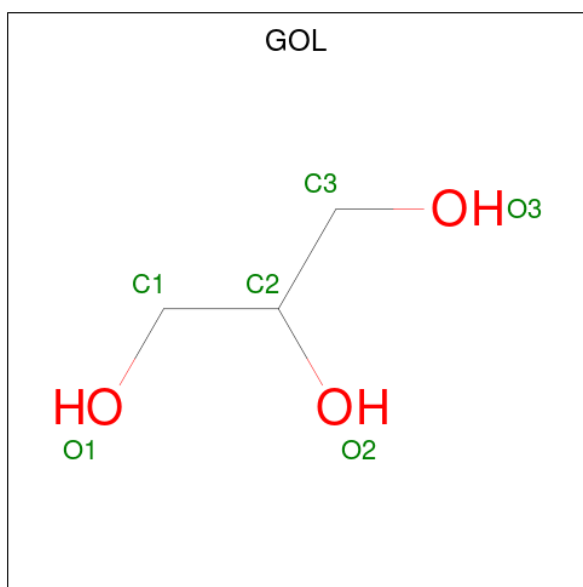
Chain	Residue	Modelled	Actual	Comment	Reference
E	358	ASN	ASP	engineered mutation	UNP Q9JJX7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	46	Total	O	0	0
			46	46		
5	C	30	Total	O	0	0
			30	30		
5	D	16	Total	O	0	0
			16	16		
5	E	24	Total	O	0	0
			24	24		

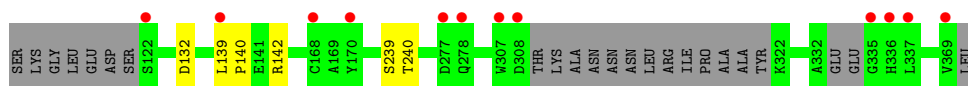
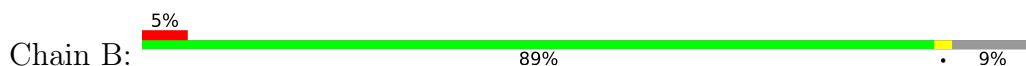
3 Residue-property plots [i](#)

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.

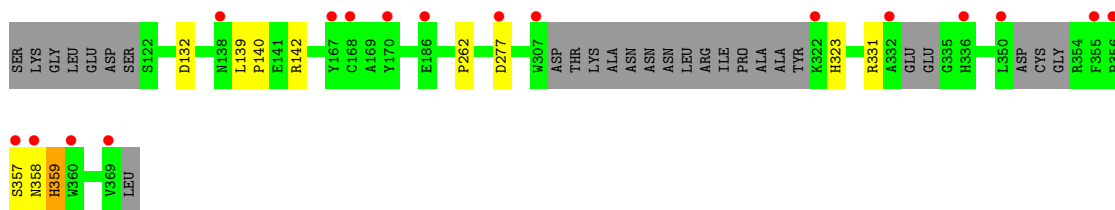
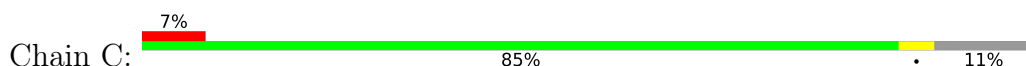
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



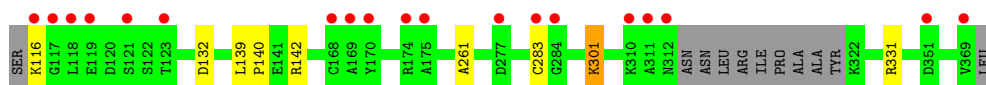
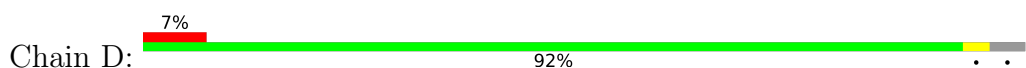
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2

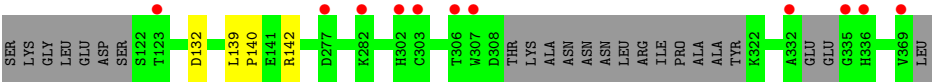


- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.44Å 114.88Å 115.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.80 49.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	49.5 (49.39-2.80) 93.3 (49.39-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.256 0.215 , 0.257	Depositor DCC
R_{free} test set	1538 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9587	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, SO4

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	0.26	0/1969	0.58	0/2663
1	B	0.27	0/1907	0.59	0/2579
1	C	0.27	0/1864	0.60	0/2518
1	D	0.27	0/1999	0.60	0/2703
1	E	0.27	0/1891	0.58	0/2556
All	All	0.27	0/9630	0.59	0/13019

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 [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	1924	0	1919	4	0
1	B	1861	0	1857	3	0
1	C	1824	0	1830	5	0
1	D	1952	0	1943	4	0
1	E	1850	0	1847	2	0
2	A	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5	0	0	0	0
3	A	6	0	8	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	0	0	0
5	B	46	0	0	0	0
5	C	30	0	0	0	0
5	D	16	0	0	0	0
5	E	24	0	0	0	0
All	All	9587	0	9404	18	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 1.

All (18) 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:327:ARG:NH2	2:A:401:SO4:O4	2.31	0.64
1:C:132:ASP:O	1:C:142:ARG:NH2	2.29	0.64
1:B:132:ASP:O	1:B:142:ARG:NH2	2.37	0.57
1:E:132:ASP:O	1:E:142:ARG:NH2	2.40	0.55
1:C:262:PRO:O	1:C:331:ARG:NH2	2.41	0.53
1:A:132:ASP:O	1:A:142:ARG:NH2	2.42	0.52
1:B:239:SER:O	1:B:240:THR:OG1	2.23	0.51
1:D:261:ALA:O	1:D:331:ARG:NH2	2.40	0.50
1:C:277:ASP:OD1	1:C:323:HIS:NE2	2.47	0.47
1:A:262:PRO:O	1:A:331:ARG:NH2	2.51	0.43
1:D:132:ASP:O	1:D:142:ARG:NH2	2.44	0.43
1:A:239:SER:O	1:A:240:THR:OG1	2.24	0.42
1:C:139:LEU:N	1:C:140:PRO:HD2	2.34	0.42
1:D:139:LEU:N	1:D:140:PRO:HD2	2.36	0.41
1:C:357:SER:C	1:C:359:HIS:H	2.28	0.41
1:D:301:LYS:H	1:D:301:LYS:HD3	1.86	0.41
1:E:139:LEU:HB3	1:E:140:PRO:HD3	2.02	0.40
1:B:139:LEU:N	1:B:140:PRO:CD	2.85	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	239/256 (93%)	227 (95%)	12 (5%)	0	100	100
1	B	228/256 (89%)	223 (98%)	5 (2%)	0	100	100
1	C	221/256 (86%)	212 (96%)	9 (4%)	0	100	100
1	D	242/256 (94%)	229 (95%)	13 (5%)	0	100	100
1	E	227/256 (89%)	220 (97%)	7 (3%)	0	100	100
All	All	1157/1280 (90%)	1111 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	214/224 (96%)	214 (100%)	0	100	100
1	B	206/224 (92%)	206 (100%)	0	100	100
1	C	202/224 (90%)	200 (99%)	2 (1%)	68	88
1	D	216/224 (96%)	213 (99%)	3 (1%)	59	85
1	E	205/224 (92%)	205 (100%)	0	100	100
All	All	1043/1120 (93%)	1038 (100%)	5 (0%)	81	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	358	ASN
1	C	359	HIS
1	D	116	LYS
1	D	283	CYS
1	D	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	B	138	ASN
1	B	236	HIS
1	B	367	ASN
1	C	161	GLN
1	C	367	ASN
1	D	138	ASN
1	D	161	GLN
1	D	204	GLN
1	D	336	HIS
1	E	161	GLN
1	E	259	GLN
1	E	323	HIS
1	E	367	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
2	SO4	E	401	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.07	0
3	GOL	A	402	-	5,5,5	0.38	0	5,5,5	0.29	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.07	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
3	GOL	A	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-O2
3	A	402	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SO4	1	0

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(Å ²)	Q<0.9
1	A	242/256 (94%)	0.04	10 (4%) 41 33	24, 42, 87, 122	1 (0%)
1	B	233/256 (91%)	-0.01	12 (5%) 33 25	23, 40, 81, 114	1 (0%)
1	C	229/256 (89%)	0.30	17 (7%) 20 15	25, 45, 97, 138	0
1	D	245/256 (95%)	0.43	19 (7%) 19 14	24, 58, 113, 169	1 (0%)
1	E	233/256 (91%)	0.27	11 (4%) 36 29	26, 48, 103, 145	0
All	All	1182/1280 (92%)	0.20	69 (5%) 29 22	23, 46, 97, 169	3 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	357	SER	5.1
1	E	303	CYS	4.9
1	C	332	ALA	4.1
1	C	336	HIS	4.0
1	B	278	GLN	3.6
1	E	307	TRP	3.6
1	C	277	ASP	3.5
1	D	117	GLY	3.4
1	A	315	LEU	3.3
1	D	118	LEU	3.3
1	E	306	THR	3.3
1	C	360	TRP	3.3
1	D	119	GLU	3.3
1	C	168	CYS	3.3
1	B	307[A]	TRP	3.2
1	A	313	ASN	3.1
1	B	168	CYS	3.1
1	E	302	HIS	3.0
1	C	350	LEU	3.0
1	D	116	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	121	SER	3.0
1	D	369	VAL	3.0
1	B	170	TYR	2.9
1	B	122	SER	2.9
1	D	170	TYR	2.8
1	E	123	THR	2.8
1	A	170	TYR	2.7
1	D	312	ASN	2.7
1	A	226	GLY	2.7
1	C	369	VAL	2.7
1	B	335	GLY	2.7
1	C	170	TYR	2.6
1	A	122	SER	2.6
1	C	167	TYR	2.6
1	A	369	VAL	2.6
1	E	335	GLY	2.5
1	E	369	VAL	2.5
1	C	355	PHE	2.5
1	E	336	HIS	2.4
1	C	307	TRP	2.4
1	D	123	THR	2.4
1	A	123	THR	2.4
1	A	260	GLU	2.3
1	D	284	GLY	2.3
1	A	307	TRP	2.3
1	B	369	VAL	2.3
1	C	358	ASN	2.3
1	B	308	ASP	2.3
1	D	283	CYS	2.3
1	C	322	LYS	2.2
1	D	351	ASP	2.2
1	B	336	HIS	2.2
1	E	277	ASP	2.2
1	D	168	CYS	2.2
1	D	175	ALA	2.2
1	E	282	LYS	2.1
1	B	139	LEU	2.1
1	D	169	ALA	2.1
1	C	138	ASN	2.1
1	B	277	ASP	2.1
1	A	276	ARG	2.1
1	C	186	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	356	PRO	2.0
1	B	337	LEU	2.0
1	D	311	ALA	2.0
1	E	332	ALA	2.0
1	D	174	ARG	2.0
1	D	277	ASP	2.0
1	D	310	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	SO4	E	401	5/5	0.69	0.13	88,88,90,90	5
2	SO4	A	401	5/5	0.70	0.14	120,122,123,123	0
2	SO4	C	401	5/5	0.79	0.14	101,102,103,103	0
4	CL	B	401	1/1	0.82	0.10	31,31,31,31	0
4	CL	C	402	1/1	0.86	0.11	45,45,45,45	0
2	SO4	D	401	5/5	0.87	0.13	79,80,81,81	0
3	GOL	A	402	6/6	0.90	0.14	32,43,44,45	6

6.5 Other polymers [i](#)

There are no such residues in this entry.