



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:21 AM UTC

PDB ID : 4G6W / pdb_00004g6w
Title : Human Thymidylate Synthase M190K with bound 4-Bromobenzene-1,2,3-triol
Authors : Celeste, L.R.; Lebioda, L.
Deposited on : 2012-07-19
Resolution : 2.30 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

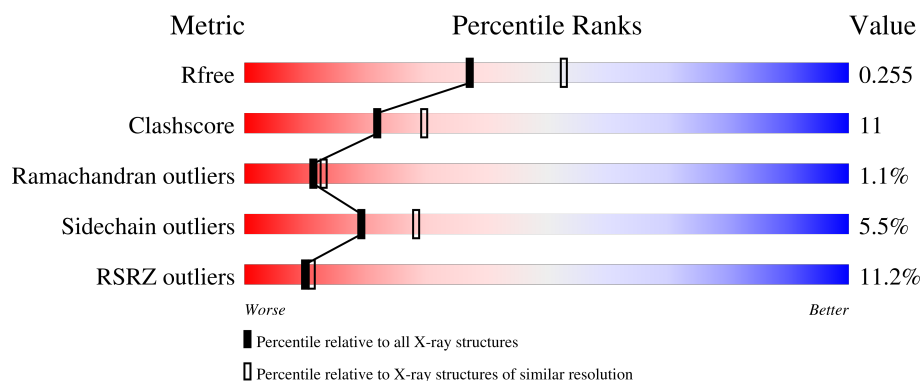
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	X	313	10% 66% 16% • • 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2222 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.

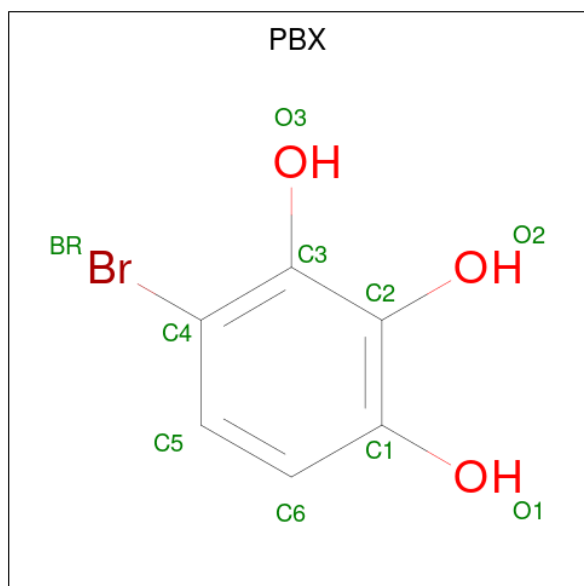
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	270	2135	1366	369	388	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

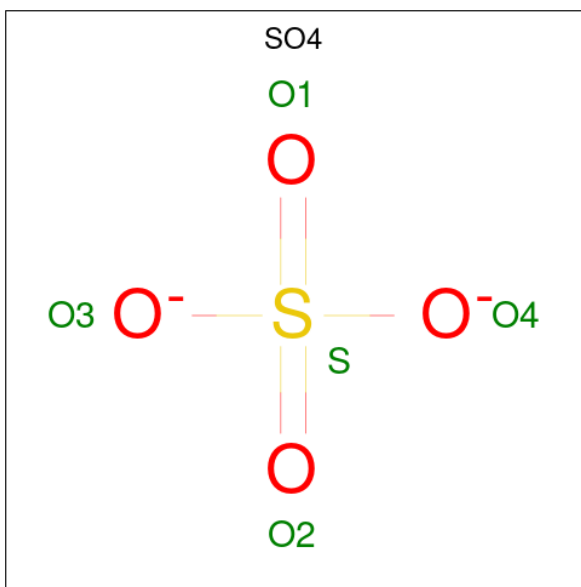
Chain	Residue	Modelled	Actual	Comment	Reference
X	190	LYS	MET	engineered mutation	UNP P04818

- Molecule 2 is 4-bromobenzene-1,2,3-triol (CCD ID: PBX) (formula: $C_6H_5BrO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
2	X	1	10	1	6	3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

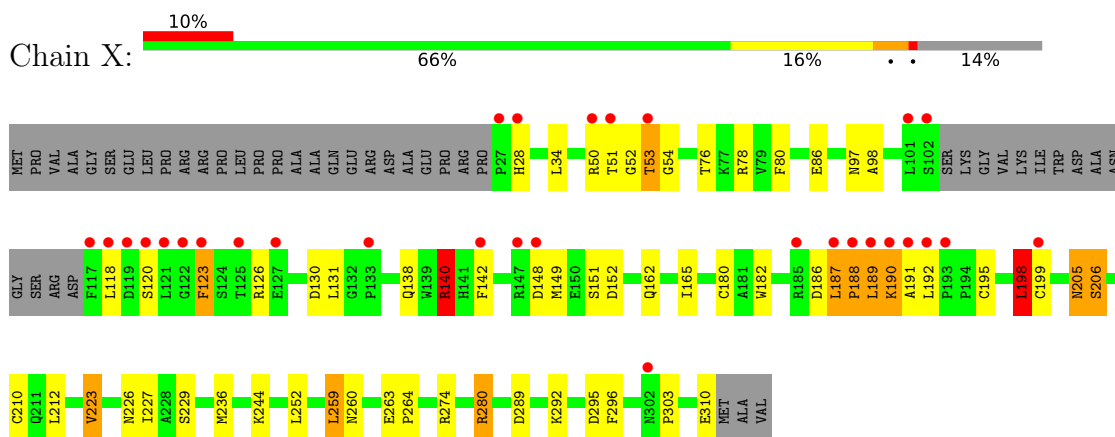


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	67	Total	O	0	0
			67	67		

- Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.85Å 95.85Å 80.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.30) 94.3 (50.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.264 0.214 , 0.255	Depositor DCC
R_{free} test set	934 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2222	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: CSD, SO4, PBX, CME

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	X	1.32	8/2171 (0.4%)	1.21	11/2946 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	223	VAL	CA-CB	-10.23	1.48	1.54
1	X	189	LEU	C-N	9.86	1.47	1.33
1	X	80	PHE	CA-C	6.15	1.61	1.52
1	X	198	LEU	C-O	-5.68	1.17	1.23
1	X	229	SER	N-CA	-5.30	1.40	1.46
1	X	162	GLN	N-CA	5.25	1.52	1.46
1	X	165	ILE	CA-C	5.24	1.59	1.52
1	X	212	LEU	CA-C	-5.11	1.46	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	190	LYS	N-CA-C	-9.49	101.01	111.36
1	X	244	LYS	CA-C-N	-6.14	113.65	119.85
1	X	244	LYS	C-N-CA	-6.14	113.65	119.85
1	X	52	GLY	N-CA-C	-5.82	106.50	114.64
1	X	205	ASN	CA-C-N	-5.38	115.55	125.02
1	X	205	ASN	C-N-CA	-5.38	115.55	125.02
1	X	206	SER	N-CA-CB	-5.21	106.00	113.65
1	X	226	ASN	N-CA-C	5.21	117.70	111.71
1	X	152	ASP	N-CA-C	5.18	116.97	108.52
1	X	140	ARG	CG-CD-NE	-5.16	100.64	112.00
1	X	28	HIS	N-CA-C	5.12	117.03	108.99

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	X	2135	0	2041	45	0
2	X	10	0	3	2	0
3	X	10	0	0	1	0
4	X	67	0	0	0	0
All	All	2222	0	2044	45	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 11.

All (45) 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:X:189:LEU:HD23	1:X:189:LEU:O	1.46	1.13
1:X:280:ARG:HG2	1:X:280:ARG:HH21	1.24	0.99
1:X:50:ARG:HH12	1:X:118:LEU:HD12	1.30	0.97
1:X:280:ARG:HH21	1:X:280:ARG:CG	1.80	0.94
1:X:50:ARG:NH1	1:X:118:LEU:HD12	1.98	0.79
1:X:260:ASN:ND2	1:X:310:GLU:HB2	1.98	0.79
1:X:189:LEU:O	1:X:189:LEU:CD2	2.30	0.76
1:X:198:LEU:C	1:X:198:LEU:HD23	2.13	0.73
1:X:187:LEU:O	1:X:188:PRO:C	2.30	0.72
1:X:236:MET:HE2	1:X:296:PHE:CZ	2.23	0.72
1:X:78:ARG:HD2	3:X:601:SO4:O4	1.91	0.71
1:X:130:ASP:CG	1:X:149:MET:HG2	2.16	0.70
1:X:54:GLY:HA3	1:X:259:LEU:HD22	1.74	0.69
1:X:186:ASP:C	1:X:188:PRO:HD2	2.17	0.69
1:X:50:ARG:HH12	1:X:118:LEU:CD1	2.05	0.66
1:X:280:ARG:CG	1:X:280:ARG:NH2	2.50	0.64
1:X:140:ARG:NH2	1:X:289:ASP:OD1	2.33	0.61
1:X:187:LEU:N	1:X:188:PRO:HD2	2.15	0.61
1:X:192:LEU:HD23	2:X:600:PBX:O2	2.01	0.60
1:X:205:ASN:O	1:X:206:SER:HB2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:280:ARG:HG2	1:X:280:ARG:NH2	2.03	0.58
1:X:260:ASN:HD22	1:X:310:GLU:HB2	1.69	0.57
1:X:182:TRP:HZ2	2:X:600:PBX:BR	2.44	0.56
1:X:98:ALA:HB2	1:X:131:LEU:HD21	1.90	0.54
1:X:236:MET:HE2	1:X:296:PHE:HZ	1.73	0.53
1:X:189:LEU:HD23	1:X:189:LEU:C	2.27	0.52
1:X:142:PHE:C	1:X:142:PHE:CD2	2.89	0.50
1:X:97:ASN:HD22	1:X:97:ASN:C	2.19	0.49
1:X:187:LEU:O	1:X:188:PRO:O	2.31	0.48
1:X:223:VAL:O	1:X:227:ILE:HG13	2.14	0.48
1:X:199:CYS:SG	1:X:210:CYS:SG	3.11	0.47
1:X:148:ASP:O	1:X:151:SER:HB3	2.14	0.47
1:X:187:LEU:HA	1:X:187:LEU:HD23	1.26	0.47
1:X:34:LEU:HD11	1:X:76:THR:HG21	1.97	0.45
1:X:263:GLU:HB2	1:X:264:PRO:HD3	1.99	0.45
1:X:187:LEU:N	1:X:188:PRO:CD	2.81	0.43
1:X:189:LEU:O	1:X:189:LEU:CG	2.66	0.43
1:X:51:THR:CG2	1:X:53:THR:OG1	2.67	0.43
1:X:123:PHE:N	1:X:123:PHE:CD2	2.86	0.43
1:X:51:THR:HG21	1:X:53:THR:OG1	2.19	0.42
1:X:198:LEU:C	1:X:198:LEU:CD2	2.87	0.42
1:X:292:LYS:N	1:X:295:ASP:OD1	2.48	0.41
1:X:190:LYS:C	1:X:192:LEU:H	2.28	0.41
1:X:263:GLU:N	1:X:264:PRO:CD	2.83	0.41
1:X:78:ARG:NH1	1:X:303:PRO:HG2	2.36	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	X	264/313 (84%)	250 (95%)	11 (4%)	3 (1%)	11 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	187	LEU
1	X	191	ALA
1	X	188	PRO

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	X	218/269 (81%)	206 (94%)	12 (6%)	19	28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	53	THR
1	X	86	GLU
1	X	120	SER
1	X	123	PHE
1	X	126	ARG
1	X	138	GLN
1	X	140	ARG
1	X	198	LEU
1	X	252	LEU
1	X	259	LEU
1	X	274	ARG
1	X	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	97	ASN
1	X	171	ASN
1	X	200	GLN
1	X	205	ASN
1	X	268	GLN

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Mol	Chain	Res	Type
1	X	270	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	X	195	1	4,7,8	3.36	2 (50%)	1,8,10	2.37	1 (100%)
1	CME	X	180	1	8,9,10	0.68	0	6,9,11	1.80	1 (16%)

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
1	CSD	X	195	1	-	1/2/6/8	-
1	CME	X	180	1	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	195	CSD	OD1-SG	-6.15	1.42	1.47
1	X	195	CSD	CB-SG	-2.06	1.67	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	180	CME	CB-SG-SD	-3.41	95.03	103.86
1	X	195	CSD	OD1-SG-CB	-2.37	101.23	105.60

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	X	195	CSD	CA-CB-SG-OD1
1	X	180	CME	SD-CE-CZ-OH
1	X	180	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	SO4	X	601	-	4,4,4	0.33	0	6,6,6	0.41	0
3	SO4	X	602	-	4,4,4	0.37	0	6,6,6	0.51	0
2	PBX	X	600	-	10,10,10	0.61	0	14,14,14	1.45	2 (14%)

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	PBX	X	600	-	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	600	PBX	BR-C4-C3	-3.13	115.30	118.80
2	X	600	PBX	BR-C4-C5	2.27	122.15	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	601	SO4	1	0
2	X	600	PBX	2	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	X	268/313 (85%)	0.61	30 (11%) 10 11	24, 44, 81, 94	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	121	LEU	5.1
1	X	192	LEU	5.0
1	X	120	SER	4.5
1	X	188	PRO	4.4
1	X	199	CYS	4.1
1	X	189	LEU	3.9
1	X	122	GLY	3.9
1	X	117	PHE	3.6
1	X	123	PHE	3.5
1	X	101	LEU	3.4
1	X	118	LEU	3.4
1	X	191	ALA	3.2
1	X	27	PRO	3.1
1	X	193	PRO	3.0
1	X	119	ASP	3.0
1	X	28	HIS	3.0
1	X	102	SER	2.8
1	X	187	LEU	2.8
1	X	190	LYS	2.8
1	X	50	ARG	2.6
1	X	51	THR	2.6
1	X	148	ASP	2.5
1	X	302	ASN	2.4
1	X	185	ARG	2.4
1	X	142	PHE	2.3
1	X	127	GLU	2.3
1	X	133	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	53	THR	2.1
1	X	125	THR	2.1
1	X	147	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	X	195	8/9	0.90	0.10	39,43,52,57	0
1	CME	X	180	10/11	0.91	0.13	38,41,61,62	0

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	PBX	X	600	10/10	0.74	0.38	45,48,50,54	10
3	SO4	X	601	5/5	0.93	0.10	63,63,65,68	0
3	SO4	X	602	5/5	0.96	0.08	60,63,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.