



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 1UPF / pdb_00001upf
Title : STRUCTURE OF THE URACIL PHOSPHORIBOSYLTRANSFERASE,
MUTANT C128V BOUND TO THE DRUG 5-FLUOROURACIL
Authors : Schumacher, M.A.; Carter, D.; Scott, D.; Roos, D.; Ullman, B.; Brennan, R.G.
Deposited on : 1998-06-17
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

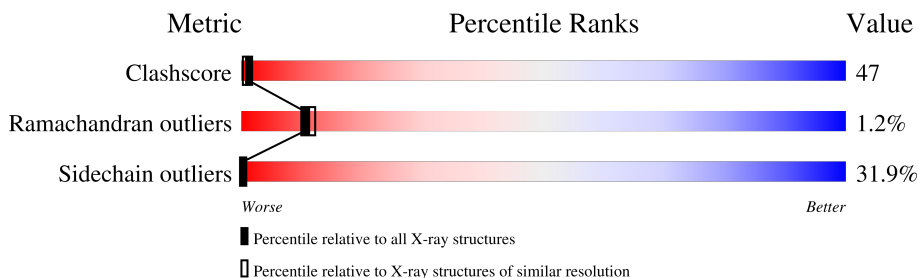
1 Overall quality at a glance

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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	35% 42% 16% 7%
1	B	224	27% 47% 21% 5%
1	C	224	32% 38% 25% .
1	D	224	32% 39% 23% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	899	-	-	X	-
2	SO4	B	599	-	-	X	-
2	SO4	B	899	-	-	X	-
2	SO4	C	799	-	-	X	-
2	SO4	C	899	-	-	X	-
2	SO4	D	599	-	X	X	-
2	SO4	D	799	-	-	X	-
2	SO4	D	899	-	-	X	-
3	URF	B	999	-	-	X	-
3	URF	C	999	-	-	X	-
3	URF	D	999	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7455 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 URACIL PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	224	1788	1146	305	324	13	0	0	0
1	C	224	1788	1146	305	324	13	0	0	0
1	B	224	1788	1146	305	324	13	0	0	0
1	A	224	1788	1146	305	324	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

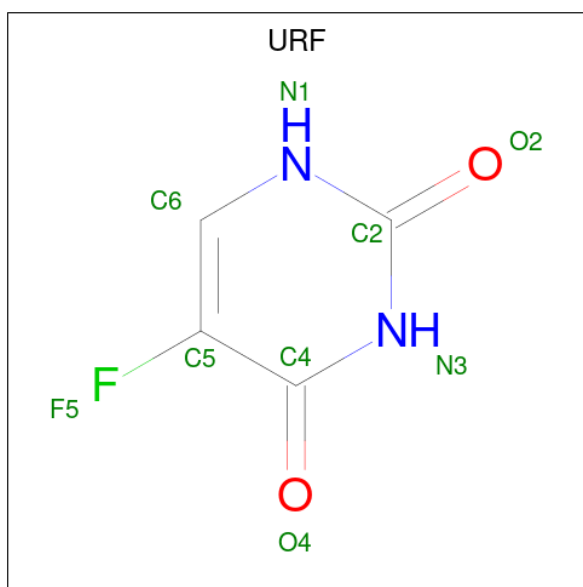
Chain	Residue	Modelled	Actual	Comment	Reference
D	84	GLN	GLU	conflict	UNP Q26998
D	128	VAL	CYS	engineered mutation	UNP Q26998
D	157	GLU	ASP	conflict	UNP Q26998
C	84	GLN	GLU	conflict	UNP Q26998
C	128	VAL	CYS	engineered mutation	UNP Q26998
C	157	GLU	ASP	conflict	UNP Q26998
B	84	GLN	GLU	conflict	UNP Q26998
B	128	VAL	CYS	engineered mutation	UNP Q26998
B	157	GLU	ASP	conflict	UNP Q26998
A	84	GLN	GLU	conflict	UNP Q26998
A	128	VAL	CYS	engineered mutation	UNP Q26998
A	157	GLU	ASP	conflict	UNP Q26998

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 5-FLUOROURACIL (CCD ID: URF) (formula: C₄H₃FN₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
3	D	1	9	4	1	2	2	0	0
3	C	1	9	4	1	2	2	0	0
3	B	1	9	4	1	2	2	0	0
3	A	1	9	4	1	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	20	20	20	0	0
4	C	93	93	93	0	0
4	B	47	47	47	0	0
4	A	47	47	47	0	0

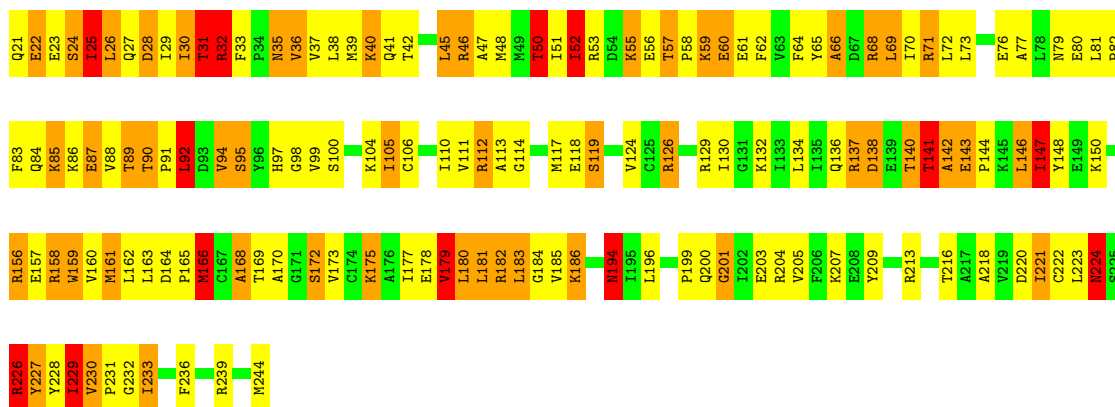
3 Residue-property plots [i](#)

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. 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. 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.

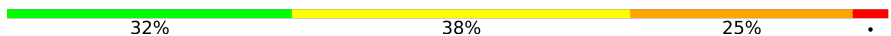
Note EDS was not executed.

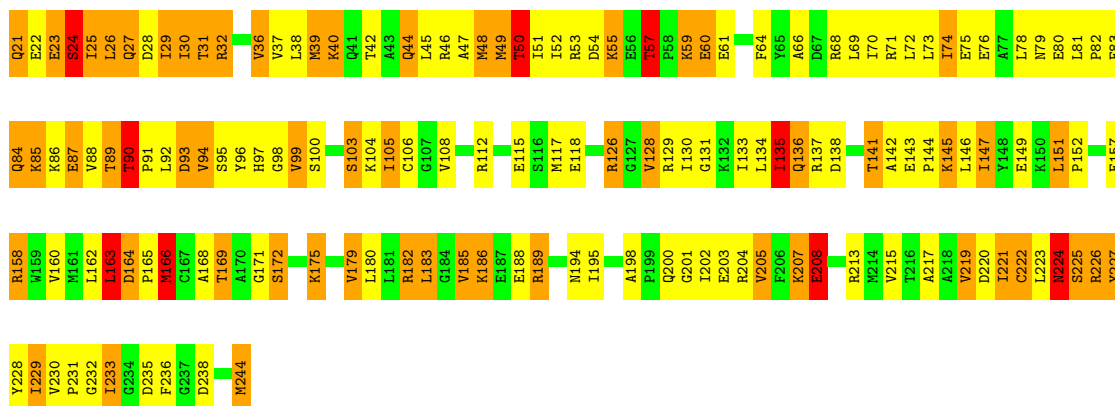
- Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE

Chain D: 



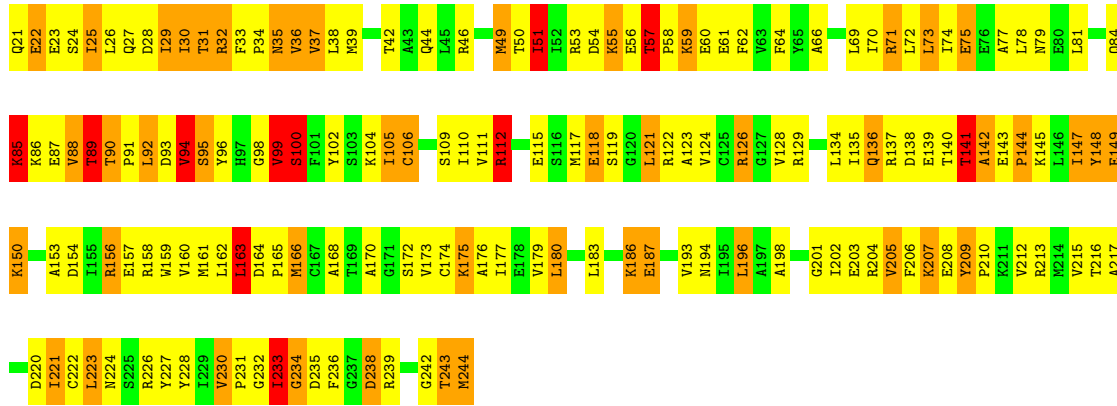
- Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE

Chain C: 

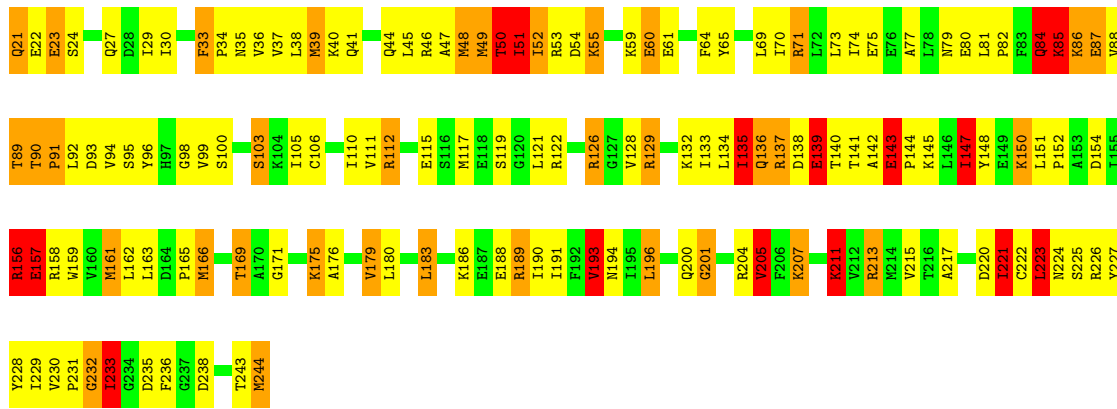


- Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE

Chain B: 



● Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.46Å 141.78Å 71.46Å 90.00° 115.03° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	86.0 (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7455	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: SO4, URF

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	1.09	0/1817	1.75	43/2450 (1.8%)
1	B	1.12	4/1817 (0.2%)	1.76	44/2450 (1.8%)
1	C	1.08	2/1817 (0.1%)	1.72	39/2450 (1.6%)
1	D	1.10	3/1817 (0.2%)	1.74	43/2450 (1.8%)
All	All	1.10	9/7268 (0.1%)	1.74	169/9800 (1.7%)

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
1	A	1	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	229	ILE	CA-CB	-11.07	1.42	1.54
1	B	73	LEU	CA-C	6.76	1.61	1.52
1	C	229	ILE	CA-CB	-6.54	1.46	1.54
1	B	209	TYR	CA-C	-5.67	1.45	1.52
1	B	110	ILE	CA-CB	-5.61	1.47	1.53

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	ASN	N-CA-CB	14.08	129.81	110.38
1	D	32	ARG	N-CA-C	11.00	123.35	111.36
1	B	100	SER	N-CA-C	10.31	125.17	110.23
1	D	22	GLU	N-CA-C	-10.07	99.85	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	GLU	N-CA-C	-9.43	97.66	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	50	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Sidechain

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	1788	0	1857	174	0
1	B	1788	0	1857	192	0
1	C	1788	0	1857	202	0
1	D	1788	0	1857	194	1
2	A	15	0	0	5	0
2	B	15	0	0	5	0
2	C	15	0	0	5	0
2	D	15	0	0	7	0
3	A	9	0	3	0	0
3	B	9	0	3	4	0
3	C	9	0	3	5	0
3	D	9	0	3	4	0
4	A	47	0	0	8	0
4	B	47	0	0	8	0
4	C	93	0	0	4	1
4	D	20	0	0	9	0
All	All	7455	0	7440	691	1

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 47.

The worst 5 of 691 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:C:138:ASP:HB3	1:C:141:THR:HG22	1.27	1.13
1:D:90:THR:HG22	1:D:92:LEU:H	1.05	1.12
2:D:599:SO4:S	2:D:599:SO4:O3	2.08	1.11
1:C:141:THR:HG23	1:C:143:GLU:H	1.13	1.10
1:B:39:MET:HE2	1:B:73:LEU:HD13	1.24	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LEU:O	4:C:1039:HOH:O[2_657]	2.01	0.19

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	222/224 (99%)	212 (96%)	8 (4%)	2 (1%)	14	17
1	B	222/224 (99%)	210 (95%)	6 (3%)	6 (3%)	4	3
1	C	222/224 (99%)	208 (94%)	14 (6%)	0	100	100
1	D	222/224 (99%)	207 (93%)	12 (5%)	3 (1%)	9	9
All	All	888/896 (99%)	837 (94%)	40 (4%)	11 (1%)	10	12

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	142	ALA
1	B	142	ALA
1	A	84	GLN
1	A	85	LYS
1	B	139	GLU

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	196/196 (100%)	140 (71%)	56 (29%)	0	0
1	B	196/196 (100%)	132 (67%)	64 (33%)	0	0
1	C	196/196 (100%)	133 (68%)	63 (32%)	0	0
1	D	196/196 (100%)	129 (66%)	67 (34%)	0	0
All	All	784/784 (100%)	534 (68%)	250 (32%)	0	0

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	188	GLU
1	A	136	GLN
1	B	57	THR
1	A	132	LYS
1	A	180	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	136	GLN
1	C	136	GLN
1	B	35	ASN
1	B	79	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](#)

16 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	SO4	B	799	-	4,4,4	0.92	0	6,6,6	1.23	1 (16%)
2	SO4	B	899	-	4,4,4	1.06	0	6,6,6	0.28	0
2	SO4	D	899	-	4,4,4	0.47	0	6,6,6	0.61	0
2	SO4	A	899	-	4,4,4	0.36	0	6,6,6	0.14	0
3	URF	C	999	-	9,9,9	1.21	2 (22%)	12,12,12	1.95	6 (50%)
2	SO4	C	899	-	4,4,4	1.24	0	6,6,6	0.78	0
2	SO4	A	599	-	4,4,4	0.82	0	6,6,6	0.18	0
3	URF	D	999	-	9,9,9	1.47	3 (33%)	12,12,12	2.20	5 (41%)
2	SO4	C	599	-	4,4,4	0.42	0	6,6,6	0.34	0
2	SO4	A	799	-	4,4,4	0.40	0	6,6,6	0.45	0
3	URF	B	999	-	9,9,9	1.07	1 (11%)	12,12,12	1.93	3 (25%)
2	SO4	D	799	-	4,4,4	0.75	0	6,6,6	0.50	0
2	SO4	C	799	-	4,4,4	0.67	0	6,6,6	0.62	0
3	URF	A	999	-	9,9,9	1.02	0	12,12,12	1.99	3 (25%)
2	SO4	D	599	-	4,4,4	3.75	1 (25%)	6,6,6	2.80	3 (50%)
2	SO4	B	599	-	4,4,4	0.45	0	6,6,6	0.36	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	URF	A	999	-	-	-	0/1/1/1
3	URF	B	999	-	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	URF	C	999	-	-	-	0/1/1/1
3	URF	D	999	-	-	-	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	599	SO4	O3-S	7.34	2.08	1.48
3	D	999	URF	C6-N1	2.56	1.40	1.36
3	D	999	URF	C2-N1	2.52	1.40	1.36
3	C	999	URF	C2-N1	2.29	1.39	1.36
3	D	999	URF	F5-C5	-2.21	1.31	1.35

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	599	SO4	O4-S-O3	-5.91	75.97	108.54
3	D	999	URF	F5-C5-C4	4.07	120.03	116.47
3	C	999	URF	C5-C6-N1	3.85	122.71	119.49
3	A	999	URF	F5-C5-C4	3.85	119.84	116.47
3	B	999	URF	C5-C6-N1	3.80	122.67	119.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	899	SO4	3	0
2	D	899	SO4	2	0
2	A	899	SO4	4	0
3	C	999	URF	5	0
2	C	899	SO4	3	0
3	D	999	URF	4	0
2	A	799	SO4	1	0
3	B	999	URF	4	0
2	D	799	SO4	2	0
2	C	799	SO4	2	0
2	D	599	SO4	3	0
2	B	599	SO4	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.