



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:09 PM UTC

PDB ID : 6FQV / pdb_00006fqv
Title : 2.60A BINARY COMPLEX OF S.AUREUS GYRASE with UNCLEAVED DNA
Authors : Bax, B.D.; Germe, T.; Basque, E.; Maxwell, A.
Deposited on : 2018-02-14
Resolution : 2.60 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

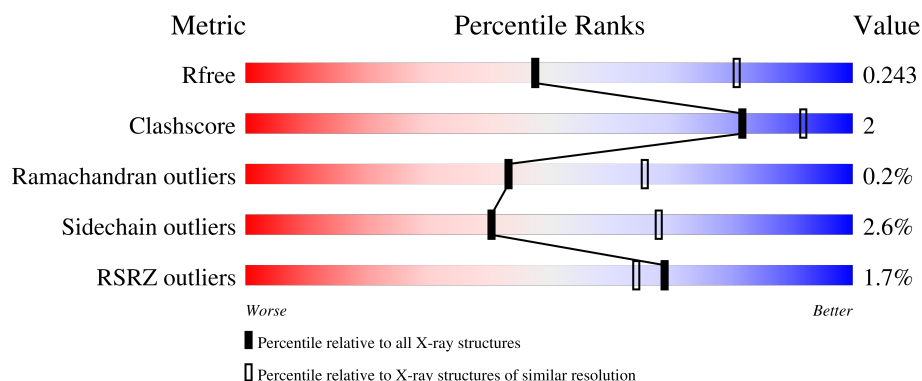
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	490	% 91% 7% ..
1	C	490	3% 88% 8% ..
1	R	490	% 90% 7% ..
1	T	490	% 88% 10% .
2	B	202	2% 88% 5% 7%

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Mol	Chain	Length	Quality of chain
2	D	202	3% 84% 9% 6%
2	S	202	2% 86% 7% 6%
2	U	202	85% 9% 5%
3	E	20	5% 90% 10%
3	F	20	10% 90% 10%
3	V	20	90% 10%
3	W	20	80% 20%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23182 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	6	0
			3833	2389	695	731	18			
1	C	473	Total	C	N	O	S	0	2	0
			3718	2316	674	712	16			
1	R	482	Total	C	N	O	S	0	5	0
			3803	2362	692	732	17			
1	T	482	Total	C	N	O	S	0	4	0
			3819	2375	704	724	16			

- Molecule 2 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	1	0
			1456	912	252	283	9			
2	D	189	Total	C	N	O	S	0	0	0
			1426	898	241	278	9			
2	S	189	Total	C	N	O	S	0	4	0
			1498	943	260	286	9			
2	U	192	Total	C	N	O	S	0	2	0
			1514	951	269	285	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	LEU	conflict	UNP P66937
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
D	409	MET	LEU	conflict	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937
S	409	MET	LEU	conflict	UNP P66937
S	544	THR	-	linker	UNP P66937

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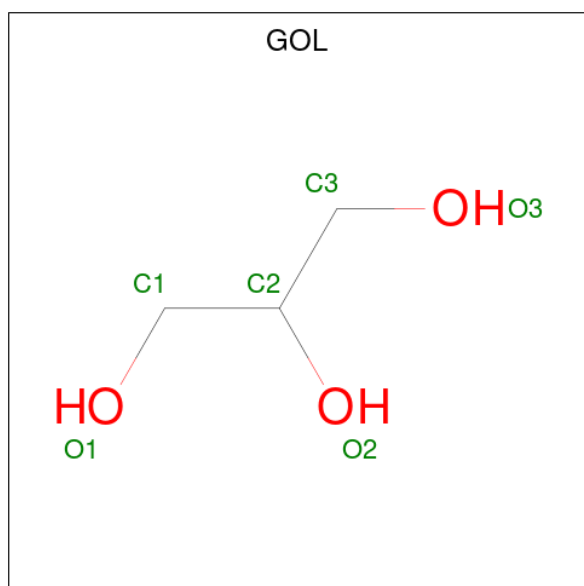
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Chain	Residue	Modelled	Actual	Comment	Reference
S	545	GLY	-	linker	UNP P66937
U	409	MET	LEU	conflict	UNP P66937
U	544	THR	-	linker	UNP P66937
U	545	GLY	-	linker	UNP P66937

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	P	0	0	0
			391	184	74	114	19			
3	F	20	Total	C	N	O	P	0	0	0
			391	184	74	114	19			
3	V	20	Total	C	N	O	P	0	0	0
			392	184	74	115	19			
3	W	20	Total	C	N	O	P	0	0	0
			393	186	74	114	19			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



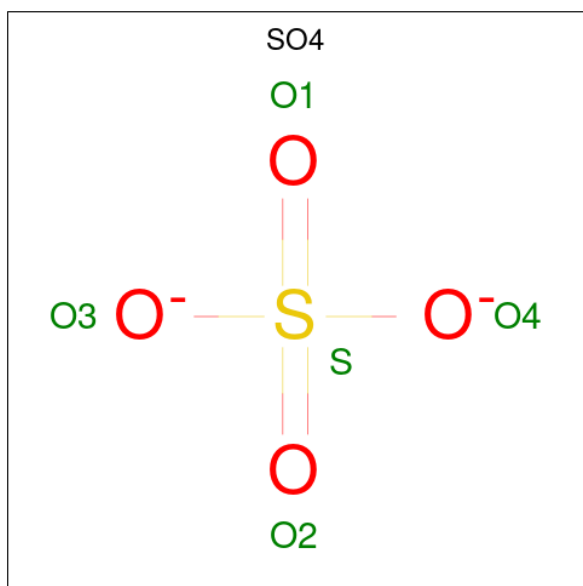
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	T	1	Total	C	O	0	0
			6	3	3		
4	T	1	Total	C	O	0	0
			6	3	3		
4	U	1	Total	C	O	0	0
			6	3	3		
4	V	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total 1	Na 1	0	0
6	T	1	Total 1	Na 1	0	0

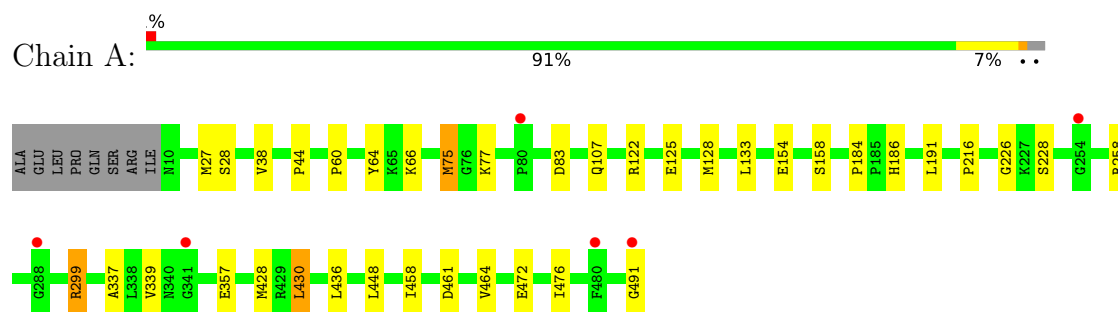
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total 84	O 84	0	1
7	B	28	Total 28	O 28	0	0
7	C	67	Total 67	O 67	0	0
7	D	19	Total 19	O 19	0	0
7	E	17	Total 17	O 17	0	0
7	F	4	Total 4	O 4	0	0
7	R	75	Total 75	O 75	0	0
7	S	32	Total 32	O 32	0	0
7	T	78	Total 79	O 79	0	1
7	U	31	Total 31	O 31	0	0
7	V	16	Total 16	O 16	0	0
7	W	18	Total 18	O 18	0	0

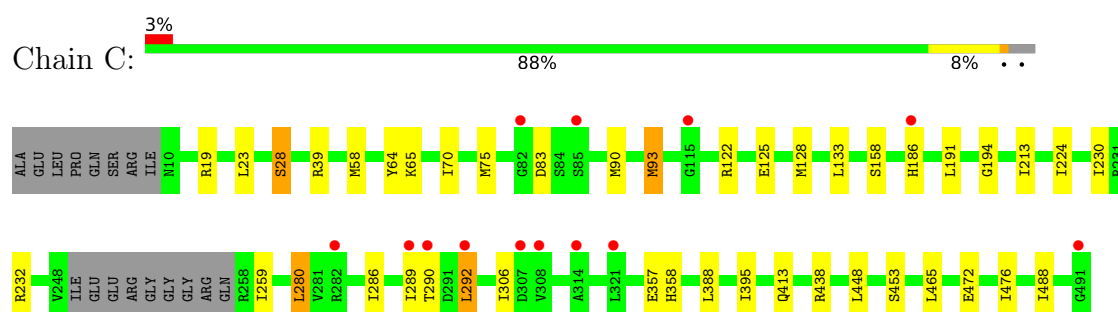
3 Residue-property plots [i](#)

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 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.

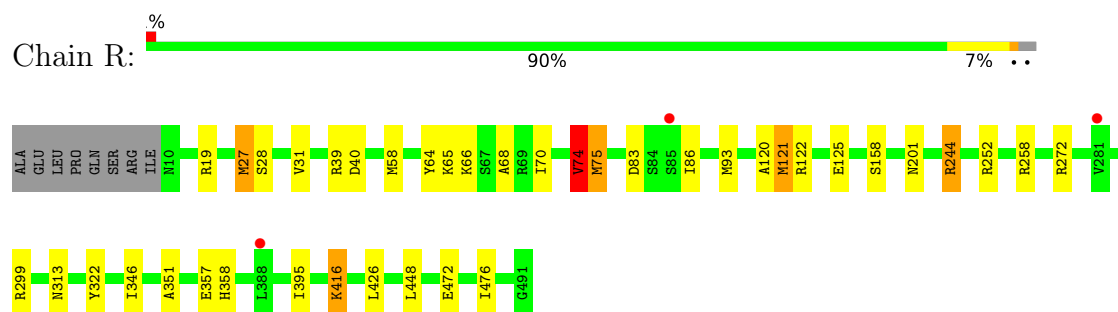
- Molecule 1: DNA gyrase subunit A



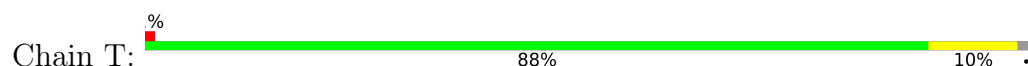
- Molecule 1: DNA gyrase subunit A

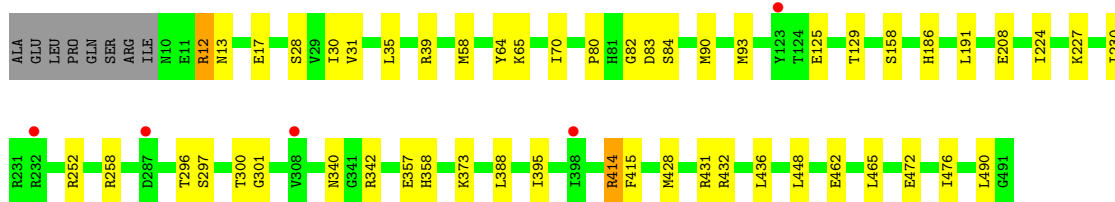


- Molecule 1: DNA gyrase subunit A

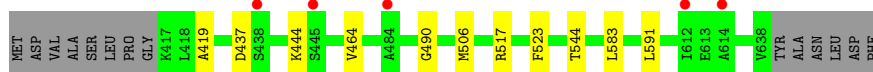
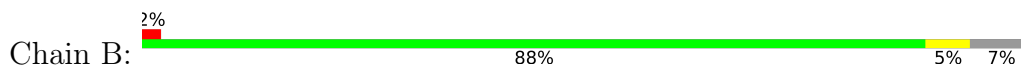


- Molecule 1: DNA gyrase subunit A

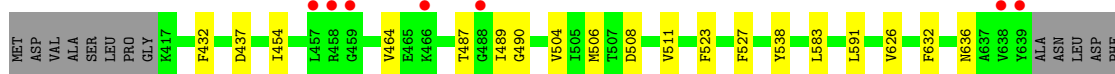
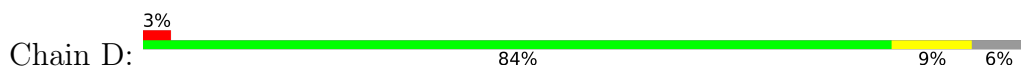




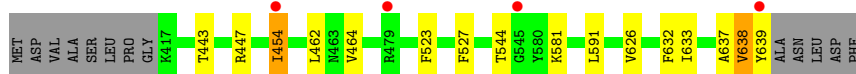
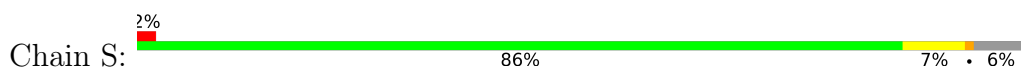
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



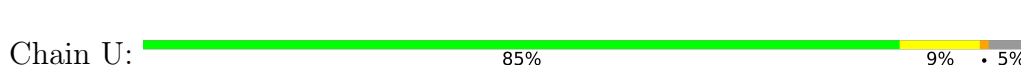
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



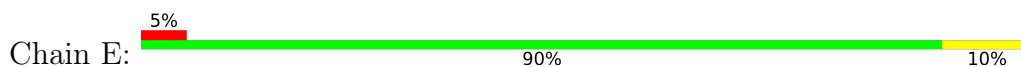
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B

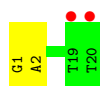


- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')





- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain V: 90% 10%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*TP*AP*CP*GP*GP*CP*CP*GP*TP*AP*CP*GP*CP*TP*T)-3')

Chain W: 80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.28Å 124.64Å 155.24Å 90.00° 95.65° 90.00°	Depositor
Resolution (Å)	19.91 – 2.60 19.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.91-2.60) 98.9 (19.91-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.236 0.206 , 0.243	Depositor DCC
R_{free} test set	5247 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.9	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	0.94	EDS
Total number of atoms	23182	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.58% 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: GOL, NA, 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	0.76	0/3884	1.35	10/5234 (0.2%)
1	C	0.77	1/3765 (0.0%)	1.35	4/5083 (0.1%)
1	R	0.77	2/3851 (0.1%)	1.34	8/5198 (0.2%)
1	T	0.77	2/3867 (0.1%)	1.34	13/5215 (0.2%)
2	B	0.79	0/1479	1.38	2/2000 (0.1%)
2	D	0.78	0/1449	1.41	3/1965 (0.2%)
2	S	0.79	1/1522 (0.1%)	1.34	0/2057
2	U	0.82	2/1538 (0.1%)	1.35	1/2075 (0.0%)
3	E	0.52	0/438	0.61	0/675
3	F	0.54	0/438	0.59	0/675
3	V	0.50	0/439	0.62	0/677
3	W	0.56	0/440	0.69	0/678
All	All	0.76	8/23110 (0.0%)	1.30	41/31532 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	586	MET	SD-CE	-8.76	1.57	1.79
2	U	454	ILE	CG1-CD1	-7.32	1.23	1.51
1	R	93	MET	SD-CE	-7.22	1.61	1.79
2	S	454	ILE	CG1-CD1	-7.22	1.23	1.51
1	T	93	MET	SD-CE	-6.30	1.63	1.79
1	R	121	MET	SD-CE	-5.74	1.65	1.79
1	C	93	MET	SD-CE	-5.47	1.65	1.79
1	T	300	THR	CA-C	5.24	1.59	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	437	ASP	CA-C-N	7.15	132.67	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	437	ASP	C-N-CA	7.15	132.67	120.72
1	A	75[A]	MET	N-CA-C	6.94	119.44	111.11
1	A	75[B]	MET	N-CA-C	6.94	119.44	111.11
1	T	208	GLU	CB-CG-CD	6.41	123.50	112.60
1	T	300	THR	CA-C-N	6.38	133.19	121.70
1	T	300	THR	C-N-CA	6.38	133.19	121.70
2	B	437	ASP	CA-C-N	5.98	130.71	120.72
2	B	437	ASP	C-N-CA	5.98	130.71	120.72
1	A	158	SER	CA-C-N	5.82	128.63	122.11
1	A	158	SER	C-N-CA	5.82	128.63	122.11
1	R	120	ALA	CA-C-N	5.77	128.80	120.38
1	R	120	ALA	C-N-CA	5.77	128.80	120.38
1	R	74	VAL	N-CA-CB	5.75	119.20	110.58
1	T	82	GLY	CA-C-N	5.74	132.50	121.54
1	T	82	GLY	C-N-CA	5.74	132.50	121.54
1	A	430	LEU	CA-C-N	5.66	128.42	120.28
1	A	430	LEU	C-N-CA	5.66	128.42	120.28
1	T	158	SER	CA-C-N	5.52	128.29	122.11
1	T	158	SER	C-N-CA	5.52	128.29	122.11
1	R	158	SER	CA-C-N	5.44	128.21	122.11
1	R	158	SER	C-N-CA	5.44	128.21	122.11
1	C	158	SER	CA-C-N	5.38	128.13	122.11
1	C	158	SER	C-N-CA	5.38	128.13	122.11
1	C	488	ILE	CA-C-N	5.37	128.46	120.95
1	C	488	ILE	C-N-CA	5.37	128.46	120.95
1	R	313	ASN	CA-CB-CG	5.33	117.93	112.60
1	T	12	ARG	CA-C-N	5.33	128.41	120.95
1	T	12	ARG	C-N-CA	5.33	128.41	120.95
1	T	129	THR	N-CA-C	-5.32	102.65	110.52
1	T	90	MET	CA-C-N	5.23	127.14	120.56
1	T	90	MET	C-N-CA	5.23	127.14	120.56
2	D	508	ASP	CA-CB-CG	5.17	117.77	112.60
1	T	84	SER	N-CA-C	5.17	117.00	111.36
2	U	508	ASP	CA-CB-CG	5.14	117.74	112.60
1	R	40	ASP	CA-CB-CG	5.07	117.67	112.60
1	R	201	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	75[A]	MET	CA-C-N	5.03	130.75	121.70
1	A	75[A]	MET	C-N-CA	5.03	130.75	121.70
1	A	75[B]	MET	CA-C-N	5.03	130.75	121.70
1	A	75[B]	MET	C-N-CA	5.03	130.75	121.70

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	3833	0	3858	20	0
1	C	3718	0	3720	20	0
1	R	3803	0	3780	19	0
1	T	3819	0	3831	19	0
2	B	1456	0	1402	4	0
2	D	1426	0	1359	10	0
2	S	1498	0	1453	13	0
2	U	1514	0	1496	11	0
3	E	391	0	209	2	0
3	F	391	0	209	1	0
3	V	392	0	213	1	0
3	W	393	0	212	4	0
4	A	6	0	8	1	0
4	C	6	0	8	0	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	R	18	0	24	0	0
4	T	12	0	16	0	0
4	U	6	0	8	0	0
4	V	6	0	8	0	0
5	A	5	0	0	0	0
5	T	5	0	0	0	0
6	R	1	0	0	0	0
6	T	1	0	0	0	0
7	A	84	0	0	0	0
7	B	28	0	0	1	0
7	C	67	0	0	0	0
7	D	19	0	0	0	0
7	E	17	0	0	0	0
7	F	4	0	0	0	0
7	R	75	0	0	0	0
7	S	32	0	0	0	0
7	T	79	0	0	0	0
7	U	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	V	16	0	0	0	0
7	W	18	0	0	0	0
All	All	23182	0	21830	110	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 2.

All (110) 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:R:27[A]:MET:HE1	2:S:633:ILE:HG23	1.31	1.09
2:D:489:ILE:HD12	2:D:527:PHE:HB3	1.60	0.83
2:S:443:THR:HG22	2:S:454:ILE:HG12	1.64	0.79
2:S:447:ARG:HD3	2:S:454:ILE:CD1	2.21	0.71
1:T:64:TYR:HB3	1:T:125:GLU:HB3	1.73	0.70
2:S:637:ALA:HB1	2:S:639[A]:TYR:CE2	2.26	0.69
1:R:64:TYR:HB3	1:R:125:GLU:HB3	1.74	0.69
2:S:447:ARG:HD3	2:S:454:ILE:HD11	1.74	0.69
2:U:447:ARG:HD3	2:U:454:ILE:CD1	2.23	0.68
2:U:447:ARG:HD3	2:U:454:ILE:HD11	1.79	0.64
1:C:64:TYR:HB3	1:C:125:GLU:HB3	1.80	0.63
3:F:1:DG:H2''	3:F:2:DA:O5'	1.99	0.63
1:R:252:ARG:HD3	1:R:258:ARG:HB3	1.81	0.62
2:B:419:ALA:HB2	2:B:444:LYS:HE3	1.82	0.61
1:C:259:ILE:HD12	1:C:306:ILE:HD11	1.81	0.61
1:A:77:LYS:HB3	1:A:154:GLU:HG3	1.83	0.60
1:R:58:MET:HG2	1:R:65:LYS:HG3	1.84	0.60
1:R:122:ARG:HB3	1:T:80:PRO:HB2	1.83	0.59
2:U:419:ALA:HB2	2:U:444:LYS:HE3	1.84	0.59
2:U:505:ILE:HB	2:U:539:ILE:HD13	1.85	0.59
1:R:39:ARG:HB3	1:R:358:HIS:CD2	2.39	0.58
1:A:64:TYR:HB3	1:A:125:GLU:HB3	1.85	0.57
1:R:75:MET:HE2	1:R:83:ASP:HB3	1.87	0.56
1:A:461:ASP:O	1:A:464:VAL:HG12	2.06	0.55
1:A:461:ASP:HB3	1:A:464:VAL:HG12	1.88	0.54
1:R:395:ILE:HD13	1:T:395:ILE:HD13	1.90	0.53
1:R:74:VAL:HG22	1:R:86:ILE:HG21	1.90	0.53
1:C:292:LEU:HB2	1:C:306:ILE:HG22	1.91	0.52
2:U:583:LEU:HD23	2:U:586:MET:CE	2.39	0.52
2:U:447:ARG:HD3	2:U:454:ILE:HD12	1.92	0.52
1:R:27[A]:MET:HE1	2:S:633:ILE:CG2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:MET:SD	1:C:70:ILE:HG12	2.51	0.51
2:S:462:LEU:HD13	3:W:14:DT:H5''	1.93	0.51
1:T:58:MET:HG2	1:T:65:LYS:HG3	1.92	0.51
1:A:458:ILE:HA	1:A:464:VAL:HG13	1.93	0.51
2:U:460:LYS:HE3	7:U:823:HOH:O	2.10	0.51
1:R:58:MET:SD	1:R:70:ILE:HG12	2.51	0.50
1:T:428:MET:HG2	1:T:432[A]:ARG:HD3	1.94	0.50
1:T:12:ARG:HH11	1:T:17:GLU:HA	1.76	0.50
1:C:122:ARG:HH22	3:E:9:DG:P	2.34	0.50
1:A:226:GLY:HA2	1:A:491:GLY:HA3	1.94	0.50
2:D:432:PHE:HB2	2:D:454:ILE:HD13	1.94	0.50
1:A:128:MET:HE1	1:A:133:LEU:HD23	1.94	0.49
2:U:464:VAL:HG21	2:U:523:PHE:HA	1.95	0.49
2:S:447:ARG:HD3	2:S:454:ILE:HD12	1.91	0.49
1:T:186:HIS:HB2	1:T:191:LEU:HD11	1.95	0.48
1:A:60:PRO:HD3	1:A:128:MET:HE2	1.95	0.48
1:T:297:SER:O	1:T:301:GLY:HA2	2.14	0.48
2:B:506:MET:HE3	2:B:583:LEU:HD22	1.96	0.48
1:A:38:VAL:HG11	1:A:339:VAL:HG22	1.94	0.48
1:C:19:ARG:HE	2:D:632:PHE:HE1	1.60	0.48
2:D:506:MET:HE3	2:D:583:LEU:HD22	1.95	0.47
1:C:39:ARG:HB3	1:C:358:HIS:CD2	2.49	0.47
1:R:426:LEU:HB3	1:T:431:ARG:HB3	1.97	0.47
1:R:416:LYS:HG2	1:R:416:LYS:O	2.14	0.47
1:T:414:ARG:HD2	1:T:415:PHE:CZ	2.49	0.47
1:C:186:HIS:HB2	1:C:191:LEU:HD11	1.96	0.47
1:C:75:MET:SD	1:C:83:ASP:HB3	2.55	0.47
1:R:19:ARG:HE	2:S:632:PHE:HE1	1.63	0.47
1:T:39:ARG:HB3	1:T:358:HIS:CD2	2.50	0.47
1:A:75[A]:MET:SD	1:A:83:ASP:HB3	2.54	0.46
3:W:5:DG:H2'	3:W:5:DG:H5'	1.64	0.46
1:T:58:MET:SD	1:T:70:ILE:HG12	2.55	0.46
2:D:464:VAL:HG21	2:D:523:PHE:HA	1.97	0.46
1:T:252:ARG:HD3	1:T:258:ARG:HB3	1.96	0.46
1:R:66:LYS:HD2	1:R:122:ARG:O	2.16	0.46
1:A:38:VAL:HG12	1:A:337:ALA:HB3	1.98	0.45
2:B:517:ARG:HD3	7:B:716:HOH:O	2.15	0.45
2:S:581:LYS:HA	2:S:581:LYS:HD2	1.86	0.45
1:R:244:ARG:HD2	1:R:322:TYR:CD1	2.51	0.45
2:S:464:VAL:HG21	2:S:523:PHE:HA	1.99	0.45
2:S:626:VAL:HG11	3:W:17:DG:H3'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:583:LEU:HD23	2:U:586:MET:HE1	1.97	0.45
1:A:184:PRO:HB2	1:A:216:PRO:HB3	2.00	0.44
2:D:626:VAL:HG11	3:E:17:DG:H3'	1.99	0.44
1:T:296:THR:HA	1:T:301:GLY:O	2.16	0.44
1:C:23:LEU:HD21	2:D:636:ASN:O	2.18	0.44
1:R:68:ALA:HA	1:R:121:MET:HE3	1.99	0.44
1:C:388:LEU:HD13	1:C:438:ARG:HD3	1.99	0.43
1:A:44:PRO:HB3	4:A:501:GOL:H31	1.99	0.43
1:C:90:MET:HA	1:C:93:MET:HE3	2.01	0.43
1:C:128:MET:HE1	1:C:133:LEU:HD23	1.99	0.43
2:S:464:VAL:HB	2:S:527:PHE:HE2	1.84	0.43
2:U:464:VAL:HB	2:U:527:PHE:HE2	1.84	0.43
1:C:280:LEU:HB3	1:C:286:ILE:HG22	2.01	0.43
1:A:38:VAL:CG1	1:A:337:ALA:HB3	2.50	0.42
1:A:430:LEU:HD22	1:C:395:ILE:HD13	2.00	0.42
1:C:472:GLU:O	1:C:476:ILE:HG12	2.19	0.42
1:R:472:GLU:O	1:R:476:ILE:HG12	2.19	0.42
2:D:464:VAL:HB	2:D:527:PHE:HE2	1.84	0.42
2:B:464:VAL:HG21	2:B:523:PHE:HA	2.01	0.42
1:C:58:MET:HG2	1:C:65:LYS:HD3	2.02	0.42
1:T:472:GLU:O	1:T:476:ILE:HG12	2.19	0.41
3:V:4:DC:H2'	3:V:5:DG:C8	2.55	0.41
2:U:447:ARG:HB3	2:U:596:MET:HE1	2.02	0.41
1:C:28:SER:HB3	2:D:511:VAL:HG13	2.02	0.41
1:C:224:ILE:HG21	1:C:230:ILE:HD11	2.02	0.41
2:D:504:VAL:HG22	2:D:538:TYR:HB2	2.01	0.41
1:T:30:ILE:HG23	1:T:35:LEU:HD12	2.02	0.41
1:R:346:ILE:HD12	1:R:351:ALA:HB2	2.02	0.41
1:A:66:LYS:HD2	1:A:122:ARG:O	2.21	0.41
1:A:458:ILE:HA	1:A:464:VAL:CG1	2.51	0.41
1:C:194:GLY:HA3	1:C:213:ILE:HD11	2.02	0.41
1:T:224:ILE:HG21	1:T:230:ILE:HD11	2.02	0.41
1:T:373:LYS:HA	1:T:373:LYS:HD3	1.90	0.41
3:W:4:DC:H3'	3:W:5:DG:H5''	2.03	0.41
1:A:186:HIS:HB2	1:A:191:LEU:HD11	2.03	0.40
1:T:12:ARG:HG2	1:T:13:ASN:H	1.86	0.40
1:A:472:GLU:O	1:A:476:ILE:HG12	2.21	0.40
1:A:299:ARG:H	1:A:299:ARG:HG2	1.50	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	486/490 (99%)	475 (98%)	11 (2%)	0	100	100
1	C	471/490 (96%)	460 (98%)	11 (2%)	0	100	100
1	R	485/490 (99%)	473 (98%)	12 (2%)	0	100	100
1	T	484/490 (99%)	469 (97%)	14 (3%)	1 (0%)	43	66
2	B	187/202 (93%)	181 (97%)	5 (3%)	1 (0%)	24	46
2	D	187/202 (93%)	180 (96%)	5 (3%)	2 (1%)	11	25
2	S	190/202 (94%)	181 (95%)	7 (4%)	2 (1%)	11	25
2	U	192/202 (95%)	185 (96%)	6 (3%)	1 (0%)	24	46
All	All	2682/2768 (97%)	2604 (97%)	71 (3%)	7 (0%)	43	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	490	GLY
2	S	638[A]	VAL
2	S	638[B]	VAL
2	D	487	THR
1	T	83	ASP
2	U	640	ALA
2	D	490	GLY

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	408/423 (96%)	397 (97%)	11 (3%)	39	67
1	C	396/423 (94%)	385 (97%)	11 (3%)	38	66
1	R	402/423 (95%)	390 (97%)	12 (3%)	36	64
1	T	403/423 (95%)	390 (97%)	13 (3%)	34	62
2	B	149/168 (89%)	147 (99%)	2 (1%)	61	82
2	D	144/168 (86%)	143 (99%)	1 (1%)	76	89
2	S	154/168 (92%)	150 (97%)	4 (3%)	40	68
2	U	157/168 (94%)	152 (97%)	5 (3%)	34	62
All	All	2213/2364 (94%)	2154 (97%)	59 (3%)	40	67

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27[A]	MET
1	A	27[B]	MET
1	A	28	SER
1	A	107	GLN
1	A	228	SER
1	A	258	ARG
1	A	299	ARG
1	A	357	GLU
1	A	428	MET
1	A	436	LEU
1	A	448	LEU
2	B	544	THR
2	B	591	LEU
1	C	28	SER
1	C	232	ARG
1	C	280	LEU
1	C	289	ILE
1	C	290	THR
1	C	292	LEU
1	C	357	GLU
1	C	413	GLN
1	C	448	LEU
1	C	453	SER
1	C	465	LEU
2	D	591	LEU
1	R	27[A]	MET
1	R	27[B]	MET

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Mol	Chain	Res	Type
1	R	28	SER
1	R	31	VAL
1	R	74	VAL
1	R	75	MET
1	R	244	ARG
1	R	272	ARG
1	R	299	ARG
1	R	357	GLU
1	R	416	LYS
1	R	448	LEU
2	S	544	THR
2	S	591	LEU
2	S	638[A]	VAL
2	S	638[B]	VAL
1	T	28	SER
1	T	31	VAL
1	T	227	LYS
1	T	340	ASN
1	T	342	ARG
1	T	357	GLU
1	T	388	LEU
1	T	414	ARG
1	T	436	LEU
1	T	448	LEU
1	T	462	GLU
1	T	465	LEU
1	T	490	LEU
2	U	477	GLU
2	U	489	ILE
2	U	544	THR
2	U	591	LEU
2	U	639	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	201	ASN
1	A	324	GLN
1	A	334	ASN
1	A	358	HIS
1	A	489	GLN

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Mol	Chain	Res	Type
2	B	474	ASN
1	C	13	ASN
1	C	201	ASN
2	D	474	ASN
2	D	590	GLN
1	R	13	ASN
1	R	54	ASN
1	R	242	GLN
1	R	324	GLN
1	R	358	HIS
1	T	13	ASN
1	T	324	GLN
1	T	489	GLN
2	U	480	GLN
2	U	631	GLN
2	U	636	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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
4	GOL	T	502	-	5,5,5	0.07	0	5,5,5	0.24	0
4	GOL	V	101	-	5,5,5	0.08	0	5,5,5	0.30	0
4	GOL	A	501	-	5,5,5	0.08	0	5,5,5	0.26	0
4	GOL	R	502	-	5,5,5	0.11	0	5,5,5	0.36	0
4	GOL	C	501	-	5,5,5	0.06	0	5,5,5	0.40	0
5	SO4	T	503	-	4,4,4	0.24	0	6,6,6	0.09	0
4	GOL	T	501	-	5,5,5	0.15	0	5,5,5	0.30	0
4	GOL	R	503	-	5,5,5	0.09	0	5,5,5	0.30	0
5	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.13	0
4	GOL	E	101	-	5,5,5	0.09	0	5,5,5	0.17	0
4	GOL	R	501	-	5,5,5	0.10	0	5,5,5	0.22	0
4	GOL	U	701	-	5,5,5	0.13	0	5,5,5	0.31	0
4	GOL	F	101	-	5,5,5	0.05	0	5,5,5	0.21	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
4	GOL	T	502	-	-	0/4/4/4	-
4	GOL	V	101	-	-	0/4/4/4	-
4	GOL	A	501	-	-	0/4/4/4	-
4	GOL	R	502	-	-	0/4/4/4	-
4	GOL	C	501	-	-	2/4/4/4	-
4	GOL	T	501	-	-	0/4/4/4	-
4	GOL	R	503	-	-	0/4/4/4	-
4	GOL	E	101	-	-	0/4/4/4	-
4	GOL	R	501	-	-	0/4/4/4	-
4	GOL	U	701	-	-	0/4/4/4	-
4	GOL	F	101	-	-	0/4/4/4	-

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
4	C	501	GOL	O1-C1-C2-C3
4	C	501	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GOL	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	482/490 (98%)	0.05	6 (1%) 76 73	25, 58, 90, 129	6 (1%)
1	C	473/490 (96%)	0.21	13 (2%) 56 50	32, 60, 103, 133	2 (0%)
1	R	482/490 (98%)	-0.04	3 (0%) 85 83	27, 53, 96, 112	5 (1%)
1	T	482/490 (98%)	-0.08	5 (1%) 79 76	29, 54, 85, 104	4 (0%)
2	B	188/202 (93%)	0.39	5 (2%) 56 50	38, 72, 100, 124	1 (0%)
2	D	189/202 (93%)	0.41	7 (3%) 45 39	49, 71, 109, 127	0
2	S	189/202 (93%)	0.07	4 (2%) 63 58	38, 59, 81, 105	4 (2%)
2	U	192/202 (95%)	0.03	0 100 100	31, 57, 87, 108	2 (1%)
3	E	20/20 (100%)	0.41	1 (5%) 34 28	54, 69, 112, 120	0
3	F	20/20 (100%)	0.54	2 (10%) 12 9	56, 79, 110, 116	0
3	V	20/20 (100%)	-0.29	0 100 100	46, 57, 73, 78	0
3	W	20/20 (100%)	-0.12	0 100 100	47, 56, 71, 76	0
All	All	2757/2848 (96%)	0.09	46 (1%) 69 64	25, 59, 96, 133	24 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	ILE	5.6
1	C	292	LEU	3.8
2	D	459	GLY	3.6
1	T	123	TYR	3.4
2	B	438	SER	3.3
1	C	290	THR	3.2
1	C	85	SER	3.2
2	S	639[A]	TYR	3.1
2	B	484	ALA	3.0
2	B	612	ILE	2.9
2	D	457	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	614	ALA	2.9
1	A	80	PRO	2.8
1	R	388	LEU	2.8
1	C	282[A]	ARG	2.7
2	D	488	GLY	2.7
1	C	307	ASP	2.6
1	C	321	LEU	2.6
2	D	639	TYR	2.5
1	T	287	ASP	2.5
1	C	491	GLY	2.5
2	S	545	GLY	2.5
1	T	398	ILE	2.4
1	C	82	GLY	2.4
1	A	480	PHE	2.4
1	C	308	VAL	2.4
1	C	115	GLY	2.4
2	S	479[A]	ARG	2.3
1	C	314	ALA	2.3
1	A	341	GLY	2.3
2	S	454	ILE	2.3
1	A	288	GLY	2.3
1	T	232[A]	ARG	2.2
2	D	466	LYS	2.2
1	R	281	VAL	2.2
1	T	308	VAL	2.2
1	A	491	GLY	2.1
3	F	20	DT	2.1
2	D	638	VAL	2.1
1	R	85	SER	2.1
1	A	254	GLY	2.1
2	B	445	SER	2.0
3	F	19	DT	2.0
3	E	1	DG	2.0
1	C	186	HIS	2.0
2	D	458	ARG	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 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
4	GOL	R	503	6/6	0.66	0.13	92,94,96,97	0
4	GOL	T	502	6/6	0.69	0.22	102,104,104,104	0
5	SO4	T	503	5/5	0.74	0.09	136,137,137,137	0
4	GOL	R	502	6/6	0.77	0.13	71,75,77,78	0
4	GOL	U	701	6/6	0.80	0.11	63,64,65,66	0
5	SO4	A	502	5/5	0.80	0.13	110,111,111,111	0
4	GOL	F	101	6/6	0.80	0.21	82,86,87,88	0
4	GOL	E	101	6/6	0.81	0.15	71,73,74,74	0
4	GOL	V	101	6/6	0.81	0.23	93,94,96,96	0
4	GOL	C	501	6/6	0.85	0.17	60,66,68,70	0
4	GOL	A	501	6/6	0.88	0.11	62,70,72,72	0
6	NA	T	504	1/1	0.90	0.07	65,65,65,65	0
4	GOL	T	501	6/6	0.91	0.09	48,57,61,62	0
4	GOL	R	501	6/6	0.92	0.09	44,51,53,55	0
6	NA	R	504	1/1	0.94	0.06	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.