

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 20, 2024 - 02:00 pm GMT

PDB ID	:	7Q2W
Title	:	Mutant T91S of uridine phosphorylase from Shewanella oneidensis
Authors	:	Polyakov, K.; Safonova, T.
Deposited on	:	2021-10-26
Resolution	:	1.65  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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.65 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	$1891 \ (1.66-1.66)$
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 <=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	AAA	251	<sup>2%</sup> 75%	20%	•••
1	BBB	251	71%	21%	• •
1	CCC	251	% <b>7</b> 6%	22%	•
1	DDD	251	71%	26%	•
1	EEE	251	76%	18%	••



Mol	Chain	Length	Quality of chain		
			% •		
1	$\mathbf{FFF}$	251	71%	24%	•••

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	BBB	301[A]	-	-	Х	-
2	SO4	EEE	301	-	-	Х	-
2	SO4	FFF	303	-	-	Х	-
3	GOL	DDD	302	-	-	Х	-



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22765 atoms, of which 10920 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.

Mol	Chain	Residues			Atom	s			ZeroOcc	AltConf	Trace
1	מממ	251	Total	С	Η	Ν	0	$\mathbf{S}$	87	2	0
	עעע	201	3718	1169	1851	322	362	14	01	Δ	0
1		244	Total	С	Η	Ν	0	S	86	2	0
	ГГГ	244	3649	1146	1824	315	351	13		5	0
1		245	Total	С	Н	Ν	0	S	85	2	0
	AAA	240	3643	1145	1818	316	350	14			0
1	CCC	250	Total	С	Η	Ν	0	S	86	2	0
		230	3711	1166	1851	321	358	15	80	2	0
1	FFF	242	Total	С	Η	Ν	0	S	83	1	0
		242	3583	1126	1789	311	344	13	00	T	0
1	BBB	240	Total	С	Н	Ν	0	S	02	0	0
	I BBB	240	3542	1114	1767	307	341	13	00	0	U

• Molecule 1 is a protein called Uridine phosphorylase.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	91	SER	THR	engineered mutation	UNP Q8E9X9
FFF	91	SER	THR	engineered mutation	UNP Q8E9X9
AAA	91	SER	THR	engineered mutation	UNP Q8E9X9
CCC	91	SER	THR	engineered mutation	UNP Q8E9X9
EEE	91	SER	THR	engineered mutation	UNP Q8E9X9
BBB	91	SER	THR	engineered mutation	UNP Q8E9X9

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	DDD	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	FFF	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	1
2	FFF	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	AAA	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	EEE	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	BBB	1	Total         O         S           10         8         2	0	1
2	BBB	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	DDD	1	Total 14	$\begin{array}{c} \mathrm{C} \\ \mathrm{3} \end{array}$	Н 8	O 3	2	0
3	AAA	1	Total 14	${ m C} { m 3}$	Н 8	O 3	2	0

• Molecule 4 is URACIL (three-letter code: URA) (formula:  $C_4H_4N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	FFF	1	Total 12	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	Н 4	N 2	O 2	0	0



• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	DDD	150	Total O 150 150	0	0
5	$\mathbf{FFF}$	123	Total O 123 123	0	0
5	AAA	156	Total O 156 156	0	0
5	CCC	152	Total O 152 152	0	0
5	EEE	126	Total         O           126         126	0	0
5	BBB	132	Total         O           132         132	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: Uridine phosphorylase

• Molecule 1: Uridine phosphorylase



Chain CCC:	% 76%	22% •
A1 D2 V3 L18 A19 G23 D24	R27 131 131 131 131 131 131 131 131 131 13	A109 5110 5110 1118 M123 M123 F131 E133 C133 C133 C133 C133 C133
G151 S155 S156 F159 Y160 R165	1170           R176           M181           M182           M185           M202           M202           M202           M202           M221           M231           M231           M231           M232           M231           M232           M231           M232	E235 237 237 1241 K248 K248 A251
• Molecule 1:	: Uridine phosphorylase	
Chain EEE:	76%	18% • •
A1 73 15 15 15 13 13 13 14 14 15 15 15 15 15 15 15 15 15 15 15 15 15	M12 L18 L18 L18 L18 L29 L21 L21 L41 L41 L41 L41 L41 L41 L41 L41 L41 L4	H119 H119 E124 H130 F133 E132 C133 F133 F156 F157 F159
Y160 4163 6164 8165 8180 6183 6183	Y192 E196 E196 A197 A197 A197 A197 A197 A206 Q206 Q206 Q206 Q206 Q206 Q206 Q206 Q	
• Molecule 1:	: Uridine phosphorylase	
Chain BBB:	71%	21% • •
A1 L8 L8 K10 K10 D14 G15 G15 A16	40 102 102 102 102 103 103 103 104 104 104 104 104 104 104 104 104 104	La7 La7 Ra8 Se1 192 G102 H112 H112 H112 F120 F120 F120 F120
A127 N130 F132 E132 C133 T134 V138	D143 C151 C151 S155 S155 F177 F177 F177 F177 F177 F177 F177 F	17221 17221 1222 1215 1116 1116 1222 1222 1222 1
K248 L249 L250 A251		



## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	91.40Å $95.49$ Å $91.41$ Å	Deperitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $120.03^{\circ}$ $90.00^{\circ}$	Depositor	
$\mathbf{P}_{\text{assolution}}\left(\mathring{\boldsymbol{\lambda}}\right)$	25.00 - 1.65	Depositor	
Resolution (A)	28.55 - 1.65	EDS	
% Data completeness	$98.3\ (25.00-1.65)$	Depositor	
(in resolution range)	$98.4\ (28.55-1.65)$	EDS	
$R_{merge}$	(Not available)	Depositor	
$\mathrm{R}_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.31 (at 1.65 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0258	Depositor	
B B.	0.191 , $0.232$	Depositor	
$\mathbf{n}, \mathbf{n}_{free}$	0.197 , $0.240$	DCC	
$R_{free}$ test set	7780 reflections $(4.89%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	11.8	Xtriage	
Anisotropy	1.286	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.42, 29.1	EDS	
L-test for $twinning^2$	$< L >=0.36, < L^2>=0.19$	Xtriage	
	0.338 for -h-l,k,h		
	0.338 for l,k,-h-l		
Estimated twinning fraction	0.310 for l,-k,h	Xtriage	
	0.370 for h,-k,-h-l		
	0.308 for -h-l,-k,l		
	0.082 for H, K, L		
	0.449 for -L, -K, -H		
Departed twinning fraction	0.136 for -H-L, -K, L	Depositor	
Reported twinning fraction	0.040 for L, K, -H-L	Depositor	
	0.208 for -H-L, K, H		
	0.084 for -H, -K, H+L		
Outliers	0 of 159146 reflections	Xtriage	
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	22765	wwPDB-VP	
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, SO4, URA

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).

Mal	Chain	Bo	ond lengths	Bond angles		
Mol Chair		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	AAA	1.06	1/1866~(0.1%)	1.22	3/2536~(0.1%)	
1	BBB	1.13	8/1806~(0.4%)	1.22	2/2455~(0.1%)	
1	CCC	1.13	4/1902~(0.2%)	1.23	1/2585~(0.0%)	
1	DDD	1.13	5/1907~(0.3%)	1.23	5/2593~(0.2%)	
1	EEE	1.09	6/1830~(0.3%)	1.22	0/2488	
1	FFF	1.11	7/1869~(0.4%)	1.20	3/2542~(0.1%)	
All	All	1.11	31/11180 (0.3%)	1.22	14/15199~(0.1%)	

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	BBB	0	1
1	$\operatorname{CCC}$	0	2
1	DDD	0	1
1	EEE	0	3
All	All	0	7

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	EEE	124	GLU	CD-OE2	9.05	1.35	1.25
1	AAA	76	GLU	CD-OE2	6.93	1.33	1.25
1	BBB	124	GLU	CD-OE2	-6.88	1.18	1.25
1	CCC	80	GLN	C-O	6.88	1.36	1.23
1	FFF	76	GLU	CD-OE2	6.73	1.33	1.25
1	FFF	193	GLU	CD-OE2	-6.42	1.18	1.25
1	CCC	156	SER	CA-CB	6.22	1.62	1.52
1	BBB	124	GLU	CD-OE1	6.01	1.32	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	BBB	76	GLU	CD-OE2	5.99	1.32	1.25
1	DDD	33	GLU	CD-OE2	-5.96	1.19	1.25
1	DDD	196	SER	C-O	5.91	1.34	1.23
1	FFF	179	GLY	C-O	5.78	1.32	1.23
1	DDD	179	GLY	C-O	5.75	1.32	1.23
1	CCC	110	SER	CA-CB	-5.75	1.44	1.52
1	BBB	151	GLY	C-O	5.73	1.32	1.23
1	FFF	198	THR	C-O	5.73	1.34	1.23
1	FFF	67	GLY	C-O	-5.68	1.14	1.23
1	BBB	119	HIS	C-O	5.63	1.34	1.23
1	BBB	195	GLU	CD-OE2	-5.60	1.19	1.25
1	EEE	193	GLU	CD-OE2	-5.55	1.19	1.25
1	FFF	33	GLU	CD-OE2	-5.42	1.19	1.25
1	EEE	130	ASN	C-O	5.42	1.33	1.23
1	EEE	77	GLU	CD-OE1	-5.29	1.19	1.25
1	BBB	187	MET	C-O	5.23	1.33	1.23
1	CCC	189	VAL	C-O	5.21	1.33	1.23
1	EEE	195	GLU	CD-OE2	5.16	1.31	1.25
1	DDD	224	GLU	CD-OE2	-5.15	1.20	1.25
1	DDD	198	THR	C-O	5.06	1.32	1.23
1	FFF	133	CYS	C-O	-5.02	1.13	1.23
1	EEE	159	PHE	C-O	5.02	1.32	1.23
1	BBB	130	ASN	C-O	5.02	1.32	1.23

Continued from previous page...

All	(14)	bond	angle	outliers	are	listed	below:
-----	------	------	-------	----------	-----	--------	--------

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	DDD	209	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	DDD	165	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	FFF	172	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	CCC	195	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	DDD	227	ASP	CB-CA-C	6.10	122.60	110.40
1	DDD	176	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	DDD	112	ARG	CB-CA-C	5.92	122.24	110.40
1	AAA	200	PHE	CB-CG-CD2	5.56	124.69	120.80
1	FFF	176	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BBB	220	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	AAA	88[A]	ARG	CG-CD-NE	-5.17	100.95	111.80
1	AAA	88[B]	ARG	CG-CD-NE	-5.17	100.95	111.80
1	BBB	112	ARG	CB-CA-C	5.05	120.50	110.40
1	FFF	160	TYR	CB-CA-C	5.02	120.44	110.40



There are no chirality outliers.

Mol	Chain	$\mathbf{Res}$	Type	Group
1	BBB	214	ALA	Mainchain
1	CCC	194	MET	Mainchain
1	CCC	209	ARG	Mainchain
1	DDD	232	LYS	Peptide
1	EEE	203	CYS	Mainchain
1	EEE	44	HIS	Mainchain
1	EEE	60	VAL	Mainchain

All (7) planarity outliers are listed below:

### 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	AAA	1825	1818	1807	44	0
1	BBB	1775	1767	1758	38	1
1	CCC	1860	1851	1836	44	1
1	DDD	1867	1851	1839	54	0
1	EEE	1794	1789	1777	29	0
1	$\mathbf{FFF}$	1825	1824	1810	48	0
2	AAA	5	0	0	0	0
2	BBB	15	0	0	2	0
2	DDD	5	0	0	0	0
2	EEE	5	0	0	2	0
2	FFF	10	0	0	7	0
3	AAA	6	8	8	1	0
3	DDD	6	8	8	6	0
4	$\mathbf{FFF}$	8	4	3	1	0
5	AAA	156	0	0	10	0
5	BBB	132	0	0	12	0
5	CCC	152	0	0	9	0
5	DDD	150	0	0	14	0
5	EEE	126	0	0	4	0
5	FFF	123	0	0	4	0
All	All	11845	10920	10846	253	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 12.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:EEE:165[A]:ARG:HD2	5:EEE:401:HOH:O	1.16	1.34
1:CCC:123:MET:HE3	5:CCC:370:HOH:O	1.58	1.02
2:EEE:301:SO4:S	5:EEE:402:HOH:O	2.17	0.99
1:FFF:130:ASN:O	1:FFF:134[B]:THR:HG23	1.63	0.98
2:BBB:301[A]:SO4:O2	5:BBB:402:HOH:O	1.85	0.92
1:BBB:132:GLU:OE2	1:BBB:209:ARG:NH1	2.10	0.84
1:FFF:25:PRO:O	1:FFF:48[B]:THR:HG21	1.79	0.82
1:FFF:71:THR:O	1:FFF:75:VAL:HG23	1.81	0.81
1:AAA:155:SER:HB3	1:AAA:197:ALA:HB2	1.63	0.81
1:AAA:222:GLN:NE2	5:AAA:402:HOH:O	2.15	0.79
1:CCC:155:SER:HB3	1:CCC:197:ALA:HB2	1.64	0.78
1:CCC:195:GLU:OE1	5:CCC:303:HOH:O	2.03	0.77
1:DDD:130:ASN:HD22	1:DDD:133:CYS:H	1.34	0.76
1:BBB:81:LEU:O	5:BBB:403:HOH:O	2.03	0.76
1:FFF:195:GLU:OE1	2:FFF:303:SO4:O2	2.05	0.75
1:FFF:14:ASP:OD1	1:FFF:53:TYR:OH	2.05	0.74
1:DDD:138:VAL:O	5:DDD:402:HOH:O	2.05	0.74
1:CCC:123:MET:CE	5:CCC:370:HOH:O	2.21	0.74
1:CCC:130:ASN:HD22	1:CCC:133:CYS:H	1.37	0.72
1:CCC:194:MET:N	5:CCC:303:HOH:O	2.23	0.72
1:FFF:84:ASN:ND2	1:FFF:85:THR:OG1	2.22	0.72
1:BBB:143:ASP:OD2	1:BBB:248:LYS:NZ	2.23	0.71
1:BBB:175:ARG:NH1	2:BBB:301[A]:SO4:O2	2.23	0.71
1:FFF:88[A]:ARG:HG2	1:FFF:212:CYS:SG	2.31	0.70
1:AAA:202:MET:O	1:AAA:206:GLN:HG2	1.89	0.70
1:BBB:130:ASN:HD22	1:BBB:133:CYS:H	1.39	0.69
1:DDD:104:VAL:CG2	1:DDD:146:VAL:HG11	2.23	0.69
1:EEE:237:SER:O	1:EEE:240:SER:OG	2.10	0.69
1:DDD:155:SER:HB3	1:DDD:197:ALA:HB2	1.74	0.68
1:CCC:88[B]:ARG:HD2	5:CCC:302:HOH:O	1.82	0.68
1:CCC:88[A]:ARG:HG2	1:CCC:212:CYS:SG	2.34	0.68
1:FFF:202:MET:O	1:FFF:206:GLN:HG2	1.94	0.67
1:CCC:19:ALA:HA	1:CCC:60:VAL:O	1.94	0.67
1:AAA:185:GLN:NE2	5:AAA:409:HOH:O	2.26	0.66
1:BBB:155:SER:HB3	1:BBB:197:ALA:HB2	1.76	0.66
1:BBB:41:LEU:O	5:BBB:404:HOH:O	2.13	0.66
1:BBB:30:ARG:HG3	5:BBB:432:HOH:O	1.95	0.66
5:DDD:406:HOH:O	1:AAA:123:MET:HG2	1.94	0.66
1:DDD:240:SER:O	5:DDD:403:HOH:O	2.14	0.65
2:EEE:301:SO4:O1	5:EEE:402:HOH:O	2.04	0.65

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:DDD:194:MET:HG3	3:DDD:302:GOL:O1	1.96	0.64
1:CCC:55:ASP:OD1	5:CCC:304:HOH:O	2.15	0.64
1:EEE:130:ASN:HD22	1:EEE:133:CYS:H	1.46	0.64
1:AAA:88[A]:ARG:HD2	5:AAA:401:HOH:O	1.96	0.64
1:DDD:122:PRO:HB2	1:DDD:124:GLU:OE1	1.97	0.64
1:CCC:108:GLN:HE21	1:CCC:151:GLY:HA2	1.61	0.64
1:CCC:3:VAL:HG13	1:CCC:81:LEU:HD21	1.80	0.63
1:AAA:129:ALA:HB3	5:AAA:403:HOH:O	1.98	0.63
1:DDD:224:GLU:OE2	5:DDD:404:HOH:O	2.14	0.63
1:EEE:159:PHE:O	1:EEE:165[B]:ARG:HD2	1.99	0.63
1:CCC:202:MET:O	1:CCC:206:GLN:HG2	1.99	0.62
1:BBB:206:GLN:HG3	5:BBB:439:HOH:O	1.99	0.62
1:DDD:182:LYS:NZ	5:DDD:408:HOH:O	2.33	0.61
1:EEE:93:GLY:HA2	1:EEE:218:VAL:O	2.01	0.60
1:DDD:19:ALA:HA	1:DDD:60:VAL:O	2.00	0.60
1:BBB:93:GLY:HA2	1:BBB:218:VAL:O	2.02	0.60
1:CCC:176:ARG:NH2	5:CCC:305:HOH:O	2.28	0.60
1:BBB:130:ASN:HD21	1:BBB:132:GLU:HB3	1.68	0.59
1:DDD:141:CYS:HB2	5:DDD:402:HOH:O	2.02	0.59
1:CCC:225:ILE:HG22	1:CCC:226:PRO:O	2.01	0.59
1:EEE:24:ASP:HB3	1:EEE:27:ARG:HG3	1.84	0.59
1:BBB:134:THR:O	1:BBB:138:VAL:HG23	2.01	0.59
1:CCC:130:ASN:HD21	1:CCC:132:GLU:HB3	1.67	0.58
1:EEE:76:GLU:O	1:EEE:80:GLN:HG3	2.03	0.58
1:EEE:155:SER:HB3	1:EEE:197:ALA:HB2	1.85	0.58
1:DDD:108:GLN:HE21	1:DDD:151:GLY:HA2	1.69	0.58
1:FFF:130:ASN:HD22	1:FFF:133:CYS:H	1.50	0.58
1:BBB:84:ASN:ND2	1:BBB:85:THR:OG1	2.36	0.58
1:DDD:64:THR:OG1	1:DDD:88[B]:ARG:NH1	2.37	0.58
1:DDD:103:ASP:HA	5:DDD:520:HOH:O	2.04	0.58
1:DDD:159:PHE:HE1	3:DDD:302:GOL:H2	1.69	0.57
1:AAA:130:ASN:HD22	1:AAA:133:CYS:H	1.51	0.57
1:DDD:84:ASN:C	1:DDD:84:ASN:HD22	2.07	0.57
1:CCC:84:ASN:C	1:CCC:84:ASN:HD22	2.08	0.57
1:AAA:108:GLN:HE21	1:AAA:151:GLY:HA2	1.68	0.57
1:BBB:208:TRP:CH2	5:BBB:439:HOH:O	2.52	0.57
1:EEE:202:MET:O	1:EEE:206:GLN:HG2	2.05	0.56
4:FFF:301:URA:N1	2:FFF:303:SO4:O4	2.37	0.56
1:DDD:104:VAL:HG22	1:DDD:146:VAL:HG11	1.86	0.56
1:CCC:75:VAL:HG13	1:CCC:86:PHE:CE1	2.41	0.56
1:BBB:54:ALA:HB1	1:BBB:247:LYS:HG2	1.88	0.56



	• • • • • • • • • • • • • • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:BBB:208:TRP:HH2	5:BBB:439:HOH:O	1.88	0.56
1:AAA:108:GLN:NE2	5:AAA:405:HOH:O	2.21	0.56
1:AAA:4:PHE:HD2	1:AAA:5:HIS:CE1	2.24	0.56
1:DDD:41:LEU:HD11	1:DDD:51:LEU:HB2	1.88	0.55
1:AAA:178:ALA:HB1	5:AAA:536:HOH:O	2.06	0.55
1:AAA:129:ALA:O	5:AAA:403:HOH:O	2.18	0.55
1:BBB:83:VAL:HG12	1:BBB:86:PHE:CZ	2.41	0.55
1:FFF:8:LEU:HD21	1:FFF:49:SER:OG	2.05	0.55
1:FFF:19:ALA:HB2	1:FFF:60:VAL:CG1	2.36	0.55
1:FFF:193:GLU:HB2	2:FFF:303:SO4:O2	2.07	0.55
1:FFF:143:ASP:OD2	1:FFF:248:LYS:NZ	2.22	0.55
1:AAA:84:ASN:ND2	1:AAA:85:THR:OG1	2.39	0.54
1:DDD:130:ASN:HD21	1:DDD:132:GLU:HB3	1.73	0.54
1:DDD:130:ASN:HD22	1:DDD:133:CYS:N	2.05	0.54
1:FFF:16:ALA:HB2	1:FFF:58:PRO:HB2	1.90	0.54
1:AAA:92:THR:HA	3:AAA:302:GOL:O2	2.08	0.53
1:DDD:101:VAL:O	1:DDD:231:MET:CE	2.57	0.53
1:CCC:27:ARG:HG3	5:CCC:406:HOH:O	2.08	0.53
1:DDD:181:MET:O	1:DDD:185:GLN:HG3	2.09	0.53
1:DDD:159:PHE:CE1	3:DDD:302:GOL:H2	2.45	0.52
1:DDD:73:ILE:HD11	1:CCC:159:PHE:HB2	1.91	0.52
1:FFF:16:ALA:O	5:FFF:401:HOH:O	2.18	0.52
1:FFF:19:ALA:HB2	1:FFF:60:VAL:HG13	1.92	0.52
1:DDD:88[B]:ARG:HG2	1:DDD:212:CYS:SG	2.49	0.52
1:DDD:122:PRO:HB2	1:DDD:124:GLU:CD	2.29	0.52
1:EEE:12:MET:HB3	1:EEE:41:LEU:HD22	1.92	0.52
1:AAA:47:TYR:O	5:AAA:404:HOH:O	2.19	0.51
1:EEE:164:GLU:O	1:EEE:164:GLU:HG2	2.09	0.51
1:DDD:124:GLU:OE2	5:DDD:406:HOH:O	2.18	0.51
1:CCC:118:LEU:HD21	1:CCC:123:MET:HE2	1.91	0.51
1:DDD:163:GLN:OE1	3:DDD:302:GOL:O2	2.21	0.51
1:AAA:183:GLU:O	1:AAA:187:MET:HG3	2.11	0.51
1:CCC:237:SER:O	1:CCC:241:ILE:HG13	2.11	0.50
1:AAA:161:PRO:HG3	1:BBB:120:PHE:CE1	2.46	0.50
1:FFF:88[B]:ARG:HG2	1:FFF:212:CYS:SG	2.51	0.50
1:CCC:23:GLY:HA3	5:CCC:318:HOH:O	2.10	0.50
1:EEE:84:ASN:C	1:EEE:84:ASN:HD22	2.14	0.50
1:AAA:3:VAL:HG13	1:AAA:81:LEU:HD21	1.93	0.50
1:FFF:10:LYS:NZ	5:FFF:412:HOH:O	2.45	0.50
1:FFF:83:VAL:HG12	1:FFF:86:PHE:CZ	2.46	0.49
1:AAA:88[B]:ARG:CD	5:AAA:401:HOH:O	2.38	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:FFF:47:TYR:CE1	1:FFF:74:ALA:HB2	2.47	0.49
1:DDD:112:ARG:HD2	1:DDD:127:ALA:HB2	1.94	0.48
1:DDD:225:ILE:HG23	1:DDD:226:PRO:HD2	1.95	0.48
1:FFF:160:TYR:CB	1:FFF:161:PRO:CD	2.91	0.48
1:FFF:25:PRO:HA	1:FFF:48[B]:THR:HG22	1.95	0.48
1:FFF:72:SER:HA	1:FFF:202:MET:SD	2.54	0.48
1:FFF:160:TYR:HB2	1:FFF:161:PRO:CD	2.44	0.48
1:BBB:84:ASN:C	1:BBB:84:ASN:HD22	2.17	0.48
1:AAA:108:GLN:NE2	1:AAA:151:GLY:HA2	2.29	0.48
1:BBB:29:LYS:HB2	1:BBB:50:TYR:CZ	2.49	0.48
1:DDD:104:VAL:HG21	1:DDD:146:VAL:HG11	1.96	0.48
1:AAA:84:ASN:C	1:AAA:84:ASN:HD22	2.17	0.48
1:DDD:46:GLU:HB3	1:CCC:46:GLU:HB3	1.95	0.48
1:FFF:122:PRO:HB2	1:FFF:124:GLU:CD	2.33	0.48
1:DDD:30:ARG:NH1	5:DDD:417:HOH:O	2.46	0.47
1:CCC:67:GLY:HA2	1:CCC:194:MET:O	2.13	0.47
1:FFF:195:GLU:OE1	2:FFF:303:SO4:S	2.73	0.47
1:CCC:146:VAL:HG23	1:CCC:236:VAL:HG21	1.97	0.47
1:BBB:202:MET:O	1:BBB:206:GLN:HG2	2.15	0.47
1:FFF:19:ALA:CB	1:FFF:60:VAL:HG13	2.45	0.47
1:DDD:124:GLU:N	5:DDD:406:HOH:O	2.48	0.46
1:CCC:75:VAL:HG13	1:CCC:86:PHE:CD1	2.49	0.46
1:CCC:24:ASP:C	1:CCC:24:ASP:OD1	2.52	0.46
1:FFF:67:GLY:HA2	1:FFF:194:MET:O	2.16	0.46
1:BBB:14:ASP:OD2	1:BBB:53:TYR:OH	2.25	0.46
1:BBB:176:ARG:HG2	1:BBB:177:PHE:CD2	2.51	0.46
1:AAA:13:LEU:HD22	1:AAA:81:LEU:HB3	1.98	0.46
1:EEE:154:ALA:O	1:EEE:192:TYR:HA	2.16	0.46
1:AAA:236:VAL:O	1:AAA:240:SER:HB3	2.15	0.46
1:DDD:193:GLU:HA	3:DDD:302:GOL:H12	1.98	0.45
1:CCC:83:VAL:HG12	1:CCC:86:PHE:CZ	2.51	0.45
1:CCC:84:ASN:ND2	1:CCC:85:THR:OG1	2.49	0.45
1:DDD:29:LYS:HE3	1:DDD:33:GLU:OE2	2.17	0.45
1:FFF:195:GLU:OE2	2:FFF:303:SO4:O3	2.35	0.45
1:EEE:32:ALA:HB2	1:EEE:61:ILE:HD13	1.97	0.45
1:DDD:27:ARG:O	1:DDD:31:ILE:HG13	2.17	0.45
1:DDD:31:ILE:HA	1:DDD:34:LEU:HD12	1.99	0.45
1:DDD:206:GLN:NE2	1:CCC:170:THR:OG1	2.49	0.45
1:BBB:16:ALA:HB2	1:BBB:58:PRO:HB2	1.99	0.45
1:FFF:237:SER:O	1:FFF:241:ILE:HG13	2.17	0.45
1:AAA:76:GLU:O	1:AAA:80:GLN:HG3	2.17	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:AAA:160:TYR:HB2	1:AAA:161:PRO:HD3	1.99	0.45
1:CCC:27:ARG:CD	1:CCC:31:ILE:HD11	2.47	0.45
1:CCC:143:ASP:OD2	1:CCC:248:LYS:NZ	2.44	0.45
1:EEE:163:GLN:HG2	1:EEE:192:TYR:CG	2.52	0.45
1:AAA:130:ASN:ND2	1:AAA:133:CYS:H	2.14	0.44
1:CCC:159:PHE:HD2	1:CCC:160:TYR:CE2	2.36	0.44
1:CCC:96:GLN:HB3	1:CCC:98:HIS:CE1	2.52	0.44
1:DDD:21:VAL:HA	1:DDD:62:CYS:O	2.18	0.44
1:DDD:138:VAL:HG21	1:AAA:131:PHE:CE2	2.52	0.44
1:FFF:88[A]:ARG:NH2	5:FFF:419:HOH:O	2.50	0.44
1:EEE:237:SER:O	1:EEE:241:ILE:HG13	2.17	0.44
1:AAA:66:ILE:HG23	1:AAA:194[B]:MET:HG2	1.99	0.44
1:AAA:72:SER:HA	1:AAA:202:MET:SD	2.57	0.44
1:AAA:182:LYS:HA	1:AAA:185:GLN:OE1	2.18	0.44
1:EEE:88:ARG:NH2	5:EEE:413:HOH:O	2.44	0.44
1:EEE:132:GLU:OE1	1:EEE:209:ARG:NH1	2.51	0.44
1:BBB:8:LEU:HD13	1:BBB:13:LEU:HD11	2.00	0.44
1:FFF:167:ASP:O	1:FFF:167:ASP:OD2	2.35	0.44
1:BBB:45:ARG:NH1	5:BBB:409:HOH:O	2.43	0.44
1:DDD:19:ALA:HB2	1:DDD:60:VAL:HG13	1.98	0.43
1:FFF:44:HIS:HB3	5:FFF:416:HOH:O	2.16	0.43
1:FFF:76:GLU:O	1:FFF:80:GLN:HG3	2.18	0.43
1:EEE:19:ALA:HA	1:EEE:60:VAL:O	2.18	0.43
1:DDD:228:GLU:HG3	5:DDD:503:HOH:O	2.18	0.43
1:FFF:84:ASN:C	1:FFF:84:ASN:HD22	2.21	0.43
1:FFF:86:PHE:O	1:FFF:210:ALA:HA	2.17	0.43
1:FFF:22:PRO:O	1:FFF:63:SER:HA	2.18	0.43
1:AAA:92:THR:OG1	1:AAA:191:ASN:HB2	2.18	0.43
1:DDD:148:PRO:HD3	5:DDD:402:HOH:O	2.18	0.43
1:AAA:180:SER:O	1:AAA:183:GLU:HB2	2.17	0.43
1:CCC:3:VAL:CG1	1:CCC:81:LEU:HD21	2.48	0.43
1:BBB:102:GLY:HA2	1:BBB:234:THR:HG21	2.01	0.43
1:FFF:177:PHE:CE2	1:EEE:119:HIS:CD2	3.06	0.43
1:CCC:18:LEU:C	1:CCC:18:LEU:HD23	2.39	0.43
1:CCC:19:ALA:HB2	1:CCC:60:VAL:HG13	1.99	0.43
1:DDD:98:HIS:HB3	5:DDD:525:HOH:O	2.18	0.43
1:FFF:21:VAL:HA	1:FFF:62:CYS:O	2.18	0.43
1:AAA:176:ARG:HD3	1:AAA:177:PHE:CE2	2.54	0.43
1:AAA:8:LEU:HD23	1:AAA:12:MET:HE1	1.99	0.42
1:CCC:46:GLU:HG3	1:CCC:65:GLY:HA3	2.01	0.42
1:FFF:155:SER:HB3	1:FFF:197:ALA:HB2	2.01	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:DDD:76:GLU:O	1:DDD:80:GLN:HG3	2.19	0.42
1:DDD:114:ASP:OD2	1:DDD:117:SER:HB3	2.19	0.42
1:FFF:34:LEU:CD1	1:FFF:239:VAL:HG12	2.49	0.42
1:DDD:194:MET:CG	3:DDD:302:GOL:O1	2.66	0.42
1:FFF:46:GLU:HB3	1:EEE:46:GLU:HB3	2.01	0.42
1:EEE:6:LEU:HD23	1:EEE:6:LEU:N	2.33	0.42
1:AAA:159:PHE:HB2	1:BBB:73:ILE:HD11	2.00	0.42
1:CCC:181:MET:O	1:CCC:185:GLN:HG3	2.20	0.42
1:CCC:88[A]:ARG:NH2	1:CCC:193:GLU:OE2	2.52	0.42
1:DDD:48:THR:O	1:DDD:62:CYS:HA	2.20	0.42
1:FFF:166:TYR:O	1:FFF:171:GLY:HA2	2.20	0.42
1:FFF:69:PRO:HA	1:EEE:157:ASP:O	2.20	0.41
1:BBB:124:GLU:H	1:BBB:124:GLU:CD	2.22	0.41
1:BBB:234:THR:HG23	5:BBB:507:HOH:O	2.19	0.41
1:EEE:2:ASP:OD1	1:EEE:9:THR:HG22	2.20	0.41
1:EEE:180:SER:O	1:EEE:183:GLU:HB2	2.20	0.41
1:CCC:130:ASN:ND2	1:CCC:133:CYS:H	2.13	0.41
1:BBB:61:ILE:N	1:BBB:61:ILE:HD12	2.35	0.41
1:AAA:18:LEU:HD23	1:AAA:18:LEU:C	2.40	0.41
1:BBB:10:LYS:HE3	5:BBB:497:HOH:O	2.20	0.41
1:BBB:130:ASN:ND2	1:BBB:132:GLU:HB3	2.34	0.41
1:FFF:160:TYR:OH	1:EEE:77:GLU:OE2	2.26	0.41
1:AAA:68:GLY:N	1:AAA:69:PRO:CD	2.83	0.41
1:BBB:112:ARG:HD2	1:BBB:127:ALA:HB2	2.02	0.41
1:DDD:104:VAL:CG2	1:DDD:146:VAL:CG1	2.97	0.41
1:BBB:57:LYS:HD2	1:BBB:250:LEU:HB3	2.03	0.41
1:DDD:84:ASN:C	1:DDD:84:ASN:ND2	2.74	0.41
1:FFF:134[B]:THR:OG1	1:FFF:135:THR:N	2.54	0.41
1:AAA:49:SER:HA	1:AAA:61:ILE:O	2.21	0.41
1:EEE:8:LEU:HD23	1:EEE:12:MET:CE	2.50	0.41
1:BBB:37:ASN:ND2	5:BBB:415:HOH:O	2.53	0.41
1:EEE:18:LEU:HD12	1:EEE:85:THR:HG21	2.01	0.40
1:CCC:72:SER:HA	1:CCC:202:MET:SD	2.62	0.40
1:CCC:165:ARG:NH2	1:CCC:224:GLU:O	2.53	0.40
1:EEE:21:VAL:HA	1:EEE:62:CYS:O	2.22	0.40
1:BBB:195:GLU:OE1	5:BBB:405:HOH:O	2.21	0.40
5:DDD:487:HOH:O	1:AAA:126:PRO:HB3	2.22	0.40
1:FFF:78:LEU:O	1:FFF:81:LEU:N	2.51	0.40
1:FFF:130:ASN:HD21	1:FFF:132:GLU:HB3	1.86	0.40
1:AAA:71:THR:O	1:AAA:75:VAL:HG23	2.21	0.40
1:AAA:77:GLU:O	1:AAA:81:LEU:HG	2.21	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:236:VAL:N	5:AAA:427:HOH:O	2.55	0.40
1:DDD:218:VAL:HG22	1:DDD:219:ASN:N	2.37	0.40
1:AAA:202:MET:O	1:AAA:206:GLN:CG	2.63	0.40
1:BBB:64:THR:OG1	1:BBB:88:ARG:NH1	2.39	0.40
1:DDD:19:ALA:CB	1:DDD:60:VAL:HG13	2.50	0.40

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:CCC:228:GLU:OE1	1:BBB:185:GLN:HE21[2_646]	1.51	0.09

### 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	Perce	ntiles
1	AAA	243/251~(97%)	235~(97%)	7 (3%)	1 (0%)	34	16
1	BBB	236/251~(94%)	226 (96%)	9 (4%)	1 (0%)	34	16
1	CCC	248/251~(99%)	236 (95%)	11 (4%)	1 (0%)	34	16
1	DDD	251/251~(100%)	242 (96%)	6 (2%)	3 (1%)	13	2
1	EEE	239/251~(95%)	226 (95%)	12 (5%)	1 (0%)	34	16
1	FFF	243/251 (97%)	234 (96%)	8 (3%)	1 (0%)	34	16
All	All	1460/1506~(97%)	1399 (96%)	53 (4%)	8 (0%)	25	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	160	TYR
1	DDD	235	GLU
1	FFF	160	TYR



 $Continued \ from \ previous \ page...$ 

Mol	Chain	Res	Type
1	AAA	160	TYR
1	CCC	160	TYR
1	EEE	160	TYR
1	BBB	160	TYR
1	DDD	233	LYS

#### 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	Perce	ntiles
1	AAA	191/197~(97%)	182~(95%)	9~(5%)	26	6
1	BBB	185/197~(94%)	176~(95%)	9~(5%)	25	5
1	CCC	195/197~(99%)	190 (97%)	5(3%)	46	21
1	DDD	195/197~(99%)	188 (96%)	7 (4%)	35	11
1	EEE	187/197~(95%)	185 (99%)	2 (1%)	73	57
1	$\mathbf{FFF}$	193/197~(98%)	187 (97%)	6(3%)	40	14
All	All	1146/1182~(97%)	1108 (97%)	38 (3%)	41	12

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	13	LEU
1	DDD	39	THR
1	DDD	84	ASN
1	DDD	88[A]	ARG
1	DDD	88[B]	ARG
1	DDD	193	GLU
1	DDD	231	MET
1	FFF	84	ASN
1	FFF	88[A]	ARG
1	FFF	88[B]	ARG
1	FFF	193	GLU
1	FFF	237	SER
1	FFF	250	LEU



Mol	Chain	Res	Tvpe
1	AAA	22	PRO
1	AAA	27	ARG
1	AAA	84	ASN
1	AAA	88[A]	ARG
1	AAA	88[B]	ARG
1	AAA	126	PRO
1	AAA	193	GLU
1	AAA	237	SER
1	AAA	240	SER
1	CCC	30	ARG
1	CCC	84	ASN
1	CCC	88[A]	ARG
1	CCC	88[B]	ARG
1	CCC	193	GLU
1	EEE	84	ASN
1	EEE	193	GLU
1	BBB	29	LYS
1	BBB	30	ARG
1	BBB	39	THR
1	BBB	57	LYS
1	BBB	84	ASN
1	BBB	88	ARG
1	BBB	91	SER
1	BBB	193	GLU
1	BBB	234	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

11 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).

Mal	Turne	Chain	Dec	Tink	В	ond leng	$_{ m gths}$	B	Sond ang	gles
WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	SO4	DDD	301	-	$4,\!4,\!4$	0.18	0	6,6,6	0.51	0
2	SO4	BBB	302	-	$4,\!4,\!4$	0.38	0	6,6,6	0.11	0
2	SO4	BBB	301[B]	-	$4,\!4,\!4$	0.57	0	$6,\!6,\!6$	0.47	0
4	URA	$\mathbf{FFF}$	301	-	8,8,8	0.96	0	9,10,10	1.70	2 (22%)
3	GOL	DDD	302	-	$5,\!5,\!5$	0.50	0	$5,\!5,\!5$	0.38	0
2	SO4	FFF	303	-	$4,\!4,\!4$	0.67	0	$6,\!6,\!6$	0.34	0
3	GOL	AAA	302	-	$5,\!5,\!5$	0.19	0	$5,\!5,\!5$	0.64	0
2	SO4	AAA	301	-	$4,\!4,\!4$	0.24	0	$6,\!6,\!6$	0.23	0
2	SO4	BBB	301[A]	-	$4,\!4,\!4$	0.72	0	$6,\!6,\!6$	0.37	0
2	SO4	EEE	301	-	4,4,4	1.65	1 (25%)	6,6,6	1.24	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	URA	FFF	301	-	-	-	0/1/1/1
3	GOL	DDD	302	-	-	1/4/4/4	-
3	GOL	AAA	302	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	EEE	301	SO4	O1-S	-2.54	1.32	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	$\mathbf{FFF}$	301	URA	O2-C2-N1	2.89	125.97	122.79



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	$\mathbf{FFF}$	301	URA	O4-C4-N3	-2.88	115.08	119.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	302	GOL	O1-C1-C2-C3
3	AAA	302	GOL	C1-C2-C3-O3
3	AAA	302	GOL	O1-C1-C2-O2
3	AAA	302	GOL	O2-C2-C3-O3
3	DDD	302	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	FFF	301	URA	1	0
3	DDD	302	GOL	6	0
2	FFF	303	SO4	7	0
3	AAA	302	GOL	1	0
2	BBB	301[A]	SO4	2	0
2	EEE	301	SO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







































## 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	AAA	245/251~(97%)	0.28	4 (1%) 72 75	10, 17, 30, 57	0
1	BBB	240/251~(95%)	0.21	0 100 100	11, 17, 28, 37	0
1	CCC	250/251~(99%)	0.15	2 (0%) 86 88	9, 16, 25, 46	0
1	DDD	251/251~(100%)	0.17	0 100 100	10, 17, 28, 45	0
1	EEE	242/251~(96%)	0.14	1 (0%) 92 93	10, 17, 27, 40	0
1	FFF	244/251~(97%)	0.24	2 (0%) 86 88	9, 18, 31, 49	0
All	All	1472/1506~(97%)	0.20	9 (0%) 89 90	9, 17, 29, 57	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	236	VAL	5.8
1	AAA	228	GLU	3.5
1	AAA	229	ALA	2.9
1	CCC	234	THR	2.7
1	$\mathbf{FFF}$	91	SER	2.6
1	AAA	225	ILE	2.6
1	CCC	231	MET	2.3
1	FFF	236	VAL	2.0
1	EEE	4	PHE	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 monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	FFF	302[A]	5/5	0.83	0.25	21,22,23,30	5
2	SO4	AAA	301	5/5	0.86	0.16	35,40,46,52	0
4	URA	FFF	301	8/8	0.88	0.14	22,28,30,30	0
3	GOL	DDD	302	6/6	0.89	0.16	15,19,24,27	2
2	SO4	DDD	301	5/5	0.92	0.10	25,26,34,36	0
3	GOL	AAA	302	6/6	0.93	0.13	19,23,29,29	2
2	SO4	FFF	303	5/5	0.93	0.20	15, 16, 19, 20	5
2	SO4	EEE	301	5/5	0.94	0.11	11,14,18,20	0
2	SO4	BBB	301[A]	5/5	0.95	0.12	8,9,10,11	5
2	SO4	BBB	301[B]	5/5	0.95	0.12	8,9,10,11	5
2	SO4	BBB	302	5/5	0.95	0.10	33,38,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









































## 6.5 Other polymers (i)

There are no such residues in this entry.

