



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:43 AM GMT

PDB ID : 1E8O  
Title : CORE OF THE ALU DOMAIN OF THE MAMMALIAN SRP  
Authors : Weichenrieder, O.; Wild, K.; Strub, K.; Cusack, S.  
Deposited on : 2000-09-28  
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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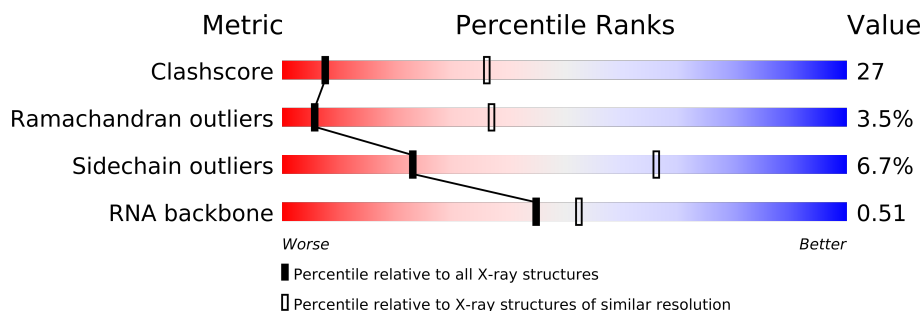
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RNA backbone	1838	1002 (3.72-2.68)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	85	
1	C	85	
2	B	106	
2	D	106	
3	E	50	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3508 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SIGNAL RECOGNITION PARTICLE 9 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	388	105	110	5			
1	C	71	Total	C	N	O	S	0	0	0
			580	369	101	105	5			

- Molecule 2 is a protein called SIGNAL RECOGNITION PARTICLE 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			600	380	104	112	4			
2	D	76	Total	C	N	O	S	0	0	0
			604	382	105	113	4			

- Molecule 3 is a RNA chain called 7SL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	50	Total	C	N	O	P	0	0	0
			1079	476	195	357	51			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	99	GDP	G	CLONING ARTEFACT	EMBL X01037
E	100	G	C	CLONING ARTEFACT	EMBL X01037
E	119	C	U	ENGINEERED MUTATION	EMBL X01037
E	148	C	G	CLONING ARTEFACT	EMBL X01037

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	2	Total	O	0	0
			2	2		
5	C	1	Total	O	0	0
			1	1		
5	D	3	Total	O	0	0
			3	3		
5	E	15	Total	O	0	0
			15	15		



Chain E: 

G99	G100	G101	C102	C103	G104	G105	G106	C107	G108	C109	G110	G111	G112	G113	G114	C115	G116	C117	G118	C119	G120	C121	C122	U123	G124	U125	U128	C129	A132	G133	A136	C137	U138	C139	G140	G141	G142	A143	G144	G145	C146	U147	C148
-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.45Å 186.62Å 189.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 3.20	Depositor
% Data completeness (in resolution range)	94.1 (47.46-3.20)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.245 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	0.50	0/619	0.75	0/832
1	C	0.42	0/589	0.66	0/791
2	B	0.50	0/604	0.74	0/804
2	D	0.39	0/608	0.65	0/809
3	E	0.57	0/1173	0.80	3/1829 (0.2%)
All	All	0.49	0/3593	0.74	3/5065 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	E	138	U	N1-C1'-C2'	5.67	121.37	114.00
3	E	137	C	C2'-C3'-O3'	5.39	122.33	113.70
3	E	132	A	C5'-C4'-C3'	-5.28	107.55	116.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	619	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	580	0	594	59	0
2	B	600	0	635	37	1
2	D	604	0	638	33	0
3	E	1079	0	544	38	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	E	5	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	1	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	E	15	0	0	0	0
All	All	3508	0	3030	179	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (179) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:38:LEU:HD12	1:C:39:CYS:H	1.17	1.04
1:A:53:THR:HG22	1:A:55:GLN:H	1.25	1.01
2:B:59:ARG:HG2	2:B:68:SER:HB3	1.44	0.99
1:C:28:VAL:HG22	1:C:41:LYS:HB3	1.44	0.98
1:A:28:VAL:HG12	2:B:29:THR:HG22	1.47	0.96
1:C:55:GLN:HA	2:D:95:LYS:HB2	1.49	0.93
1:A:3:GLN:HG3	1:A:50:VAL:HG12	1.50	0.91
2:D:61:THR:HG22	2:D:63:GLY:H	1.36	0.89
1:C:5:GLN:HG3	1:C:6:THR:H	1.40	0.83
1:C:38:LEU:HD12	1:C:39:CYS:N	1.91	0.83
2:D:4:LEU:HD22	2:D:8:GLN:HG2	1.60	0.83
1:A:21:ASP:OD2	1:A:24:LYS:HB2	1.79	0.81
1:A:28:VAL:HG12	2:B:29:THR:CG2	2.13	0.77
1:C:53:THR:HG21	1:C:58:ASP:HB2	1.67	0.77
1:C:70:MET:HB2	2:D:30:LEU:HD21	1.65	0.76
1:A:53:THR:CG2	1:A:55:GLN:H	1.98	0.76
1:C:56:ALA:HB2	2:D:95:LYS:O	1.87	0.74
1:A:46:LEU:HD12	1:A:47:VAL:N	2.02	0.73
1:A:53:THR:HG22	1:A:54:ASP:N	2.02	0.73
1:A:46:LEU:CD1	1:A:47:VAL:HG23	2.20	0.72
3:E:132:A:O2'	3:E:133:G:H8	1.72	0.71
1:C:28:VAL:CG2	1:C:41:LYS:HB3	2.19	0.70
1:C:15:GLU:O	1:C:19:LEU:HG	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:2:VAL:HG23	3:E:129:C:OP1	1.92	0.70
1:A:30:LYS:HD2	2:B:27:TYR:CE1	2.27	0.69
3:E:132:A:HO2'	3:E:133:G:H8	1.37	0.69
1:C:32:ARG:HH21	3:E:122:C:P	2.17	0.67
2:B:88:ARG:HD2	5:B:2002:HOH:O	1.94	0.67
1:A:69:LEU:O	1:A:73:MET:HG3	1.95	0.67
1:C:5:GLN:HG3	1:C:6:THR:N	2.09	0.67
2:B:86:LEU:HD23	2:B:86:LEU:C	2.16	0.66
1:A:17:LEU:HD12	1:A:49:LEU:HD11	1.78	0.65
1:A:43:THR:HG22	1:A:48:CYS:SG	2.36	0.65
1:A:53:THR:HG22	1:A:55:GLN:N	2.07	0.65
2:B:59:ARG:HG2	2:B:68:SER:CB	2.24	0.64
3:E:132:A:O2'	3:E:133:G:C8	2.50	0.64
3:E:148:C:C5'	3:E:148:C:H6	2.11	0.64
2:D:76:VAL:O	2:D:80:GLN:HG3	1.99	0.63
2:B:80:GLN:HG3	2:B:81:MET:N	2.13	0.63
1:A:55:GLN:HB3	1:A:57:GLN:HG2	1.79	0.63
1:A:30:LYS:HD2	2:B:27:TYR:HE1	1.64	0.62
3:E:121:C:O2'	3:E:122:C:H5'	1.99	0.62
1:C:53:THR:HG22	1:C:54:ASP:N	2.14	0.62
1:A:53:THR:CG2	1:A:54:ASP:N	2.63	0.62
1:A:28:VAL:CG1	2:B:29:THR:HG22	2.26	0.61
3:E:114:G:O2'	3:E:115:C:H5'	2.00	0.61
2:B:72:SER:O	2:B:76:VAL:HG22	2.00	0.61
3:E:110:G:C2'	3:E:111:G:H5'	2.31	0.61
1:C:74:VAL:HG11	2:D:76:VAL:HG11	1.81	0.61
3:E:137:C:O2	3:E:137:C:H3'	2.01	0.60
2:D:19:LYS:HG2	2:D:19:LYS:O	2.02	0.60
3:E:122:C:O2'	3:E:123:U:H5'	2.01	0.60
1:A:60:LYS:HE3	2:B:88:ARG:NH2	2.17	0.59
2:D:4:LEU:HD11	2:D:12:GLU:HG3	1.83	0.59
1:C:12:ARG:CG	1:C:13:ALA:N	2.65	0.59
3:E:138:U:H4'	3:E:139:C:OP2	2.01	0.59
1:C:46:LEU:O	1:C:47:VAL:HG13	2.02	0.59
3:E:141:G:O2'	3:E:142:G:H5'	2.02	0.59
2:D:4:LEU:HD22	2:D:8:GLN:CG	2.29	0.59
2:B:73:SER:HA	2:B:76:VAL:CG2	2.33	0.59
1:A:60:LYS:HE3	2:B:88:ARG:HH21	1.68	0.58
2:B:80:GLN:HE21	3:E:113:G:H8	1.50	0.57
1:A:46:LEU:HD12	1:A:47:VAL:HG23	1.86	0.57
1:C:32:ARG:O	1:C:32:ARG:HG2	2.04	0.57
2:B:13:LEU:HD11	2:B:17:PHE:HE1	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:148:C:H5''	3:E:148:C:H6	1.69	0.57
1:C:12:ARG:HG2	1:C:13:ALA:N	2.20	0.56
1:C:12:ARG:HG2	1:C:13:ALA:H	1.68	0.56
3:E:110:G:O2'	3:E:111:G:H5'	2.04	0.56
1:A:46:LEU:HD13	1:A:47:VAL:HG23	1.88	0.56
1:C:29:LEU:HD13	1:C:40:VAL:HG22	1.87	0.56
1:A:74:VAL:O	1:A:74:VAL:HG22	2.06	0.56
1:C:13:ALA:O	1:C:16:LYS:HB3	2.05	0.56
1:C:53:THR:HG21	1:C:58:ASP:CB	2.34	0.56
1:C:7:TRP:CD1	1:C:61:LYS:HD3	2.42	0.55
1:C:29:LEU:HD11	1:C:38:LEU:HD11	1.86	0.55
1:A:44:ASP:HB3	1:A:46:LEU:CD1	2.36	0.55
1:C:5:GLN:CG	1:C:6:THR:H	2.11	0.55
1:A:60:LYS:CD	2:B:88:ARG:HH21	2.20	0.54
1:A:17:LEU:CD1	1:A:49:LEU:HD11	2.36	0.54
2:D:61:THR:HG22	2:D:63:GLY:N	2.16	0.54
1:C:5:GLN:O	1:C:9:GLU:N	2.34	0.54
3:E:102:C:O2'	3:E:103:C:H5'	2.08	0.54
2:D:59:ARG:NH2	3:E:125:U:OP2	2.41	0.54
2:B:27:TYR:O	2:B:60:ALA:HA	2.07	0.53
2:D:30:LEU:HD13	2:D:58:LEU:HD13	1.90	0.53
1:C:65:PHE:CZ	1:C:69:LEU:HD11	2.44	0.53
3:E:105:G:O2'	3:E:106:G:H5'	2.08	0.53
1:C:32:ARG:NH2	2:D:25:SER:OG	2.42	0.53
2:D:92:ASP:OD1	2:D:92:ASP:O	2.27	0.53
1:A:54:ASP:O	2:B:95:LYS:HG2	2.08	0.53
2:B:16:LEU:HD22	2:B:62:ASP:HB3	1.91	0.52
2:D:34:ASP:CG	2:D:35:GLY:H	2.13	0.52
1:C:40:VAL:HG21	1:C:62:ILE:HG23	1.91	0.52
2:D:5:GLU:O	2:D:6:SER:C	2.48	0.52
1:C:40:VAL:CG2	1:C:62:ILE:HG23	2.40	0.52
2:D:7:GLU:O	2:D:8:GLN:C	2.47	0.51
1:C:33:HIS:CD2	2:D:21:ARG:HG3	2.46	0.51
1:C:70:MET:CB	2:D:30:LEU:HD21	2.38	0.51
2:D:56:CYS:SG	2:D:71:VAL:HB	2.50	0.51
2:D:28:ILE:HA	2:D:59:ARG:O	2.11	0.51
1:A:73:MET:SD	2:B:56:CYS:HB2	2.52	0.50
2:B:30:LEU:HD13	2:B:58:LEU:HD13	1.93	0.50
1:C:32:ARG:HH22	3:E:121:C:H5''	1.76	0.50
1:A:7:TRP:HZ2	1:A:65:PHE:HB2	1.75	0.50
1:A:53:THR:HG21	1:A:58:ASP:OD2	2.11	0.50
2:B:4:LEU:HD22	2:B:8:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:LEU:CD2	1:A:62:ILE:HD12	2.42	0.49
3:E:107:C:O2'	3:E:108:G:H5'	2.12	0.49
1:A:29:LEU:HD21	1:A:38:LEU:HD11	1.93	0.49
3:E:119:C:O2'	3:E:120:G:H5'	2.12	0.49
3:E:142:G:O2'	3:E:143:A:H5'	2.13	0.49
1:C:44:ASP:HB3	1:C:47:VAL:HG23	1.95	0.49
2:B:13:LEU:HD11	2:B:17:PHE:CE1	2.47	0.49
3:E:121:C:C2'	3:E:122:C:H5'	2.43	0.49
3:E:147:U:H2'	3:E:148:C:H5''	1.94	0.49
3:E:145:G:O2'	3:E:146:C:H5'	2.13	0.49
1:C:34:SER:C	1:C:36:GLY:N	2.65	0.48
1:A:46:LEU:HD12	1:A:47:VAL:H	1.76	0.48
1:C:5:GLN:O	1:C:9:GLU:HB2	2.14	0.48
1:A:60:LYS:CE	2:B:88:ARG:HH21	2.27	0.47
1:C:34:SER:O	1:C:36:GLY:N	2.47	0.47
2:B:86:LEU:HD23	2:B:86:LEU:O	2.13	0.47
2:D:4:LEU:HB3	2:D:8:GLN:HB3	1.95	0.47
1:A:21:ASP:CG	1:A:21:ASP:O	2.53	0.47
1:C:5:GLN:O	1:C:9:GLU:CB	2.63	0.47
2:D:4:LEU:HD13	2:D:8:GLN:HG3	1.95	0.47
1:C:32:ARG:HH11	1:C:32:ARG:HG3	1.79	0.47
2:D:30:LEU:HD12	2:D:31:LYS:H	1.79	0.46
2:B:87:LEU:HD22	2:B:91:MET:CE	2.45	0.46
1:C:53:THR:CG2	1:C:54:ASP:N	2.77	0.46
1:A:17:LEU:HD23	1:A:17:LEU:O	2.16	0.46
2:B:15:ARG:O	2:B:19:LYS:HG3	2.15	0.46
1:C:44:ASP:HB3	1:C:47:VAL:CG2	2.46	0.46
3:E:105:G:C2'	3:E:106:G:H5'	2.47	0.45
1:C:26:ARG:HH11	1:C:26:ARG:HG2	1.82	0.45
1:A:53:THR:CG2	1:A:54:ASP:H	2.28	0.45
3:E:128:U:C2	3:E:129:C:C5	3.05	0.45
1:A:38:LEU:HD21	1:A:62:ILE:HD12	1.98	0.45
1:C:68:GLN:O	1:C:71:ARG:N	2.50	0.45
2:B:94:LEU:HD12	2:B:94:LEU:N	2.32	0.45
1:C:29:LEU:CD1	1:C:38:LEU:HD11	2.46	0.45
3:E:148:C:H5''	3:E:148:C:C6	2.50	0.45
1:C:27:VAL:HG13	2:D:30:LEU:HB3	2.00	0.44
1:C:37:ASN:CA	2:D:94:LEU:HD11	2.47	0.44
1:C:29:LEU:CD1	1:C:40:VAL:HG22	2.47	0.44
3:E:148:C:C5'	3:E:148:C:C6	2.96	0.44
3:E:116:G:H2'	3:E:117:C:H5'	1.98	0.44
1:C:70:MET:HE2	2:D:30:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:ARG:O	1:A:13:ALA:C	2.57	0.43
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.75	0.43
1:C:32:ARG:NH1	1:C:32:ARG:HG3	2.33	0.43
1:C:46:LEU:C	1:C:47:VAL:HG22	2.39	0.43
1:C:61:LYS:HE2	1:C:61:LYS:HB3	1.71	0.43
1:C:32:ARG:NH2	3:E:121:C:H5'	2.33	0.43
1:A:73:MET:HE1	2:B:31:LYS:HA	2.01	0.43
1:C:37:ASN:N	2:D:94:LEU:HD11	2.34	0.43
2:B:22:THR:HG22	2:B:23:SER:N	2.34	0.43
1:A:53:THR:HG22	1:A:54:ASP:H	1.82	0.42
1:C:27:VAL:CG1	2:D:30:LEU:HB3	2.49	0.42
2:B:87:LEU:HD22	2:B:91:MET:HE2	2.01	0.42
2:D:7:GLU:O	2:D:10:LEU:N	2.47	0.42
3:E:138:U:O2	3:E:138:U:C2'	2.67	0.42
1:A:60:LYS:HG3	2:B:88:ARG:HH21	1.83	0.42
3:E:138:U:O2	3:E:138:U:H2'	2.19	0.42
2:D:7:GLU:O	2:D:9:PHE:N	2.52	0.42
1:C:5:GLN:HA	1:C:5:GLN:OE1	2.20	0.42
2:B:94:LEU:N	2:B:94:LEU:CD1	2.84	0.41
1:C:63:GLU:C	1:C:63:GLU:CD	2.78	0.41
3:E:114:G:C2'	3:E:115:C:H5'	2.49	0.41
2:B:22:THR:HG22	2:B:23:SER:OG	2.21	0.41
1:C:60:LYS:O	1:C:64:LYS:HG3	2.20	0.41
1:C:63:GLU:O	1:C:66:HIS:HB3	2.20	0.41
3:E:110:G:H2'	3:E:111:G:H5'	2.02	0.41
2:B:58:LEU:HD12	2:B:58:LEU:HA	1.96	0.41
3:E:148:C:H5'	3:E:148:C:H6	1.86	0.41
2:B:8:GLN:HA	2:B:8:GLN:OE1	2.21	0.40
1:C:69:LEU:O	1:C:73:MET:HG3	2.21	0.40
3:E:116:G:C2'	3:E:117:C:H5'	2.52	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	Distance(Å)	Clash(Å)
2:B:7:GLU:OE1	2:B:7:GLU:OE1[3_655]	1.99	0.21

## 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	72/85 (85%)	61 (85%)	9 (12%)	2 (3%)	8	44
1	C	69/85 (81%)	57 (83%)	9 (13%)	3 (4%)	4	30
2	B	71/106 (67%)	61 (86%)	9 (13%)	1 (1%)	16	66
2	D	72/106 (68%)	63 (88%)	5 (7%)	4 (6%)	3	23
All	All	284/382 (74%)	242 (85%)	32 (11%)	10 (4%)	6	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	SER
1	C	47	VAL
2	D	6	SER
2	D	7	GLU
2	D	8	GLN
1	A	46	LEU
2	B	23	SER
1	C	35	ASP
2	D	93	GLY
1	A	21	ASP

### 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	67/77 (87%)	64 (96%)	3 (4%)	38	81
1	C	64/77 (83%)	58 (91%)	6 (9%)	13	45
2	B	69/96 (72%)	63 (91%)	6 (9%)	15	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	69/96 (72%)	66 (96%)	3 (4%)	40	81
All	All	269/346 (78%)	251 (93%)	18 (7%)	23	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	63	GLU
1	A	66	HIS
2	B	2	VAL
2	B	22	THR
2	B	32	LYS
2	B	56	CYS
2	B	76	VAL
2	B	80	GLN
1	C	26	ARG
1	C	38	LEU
1	C	39	CYS
1	C	47	VAL
1	C	63	GLU
1	C	74	VAL
2	D	20	CYS
2	D	54	ASN
2	D	76	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	68	GLN
2	B	85	ASN
2	D	85	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	48/50 (96%)	11 (22%)	2 (4%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	101	G
3	E	104	G
3	E	128	U
3	E	129	C
3	E	132	A
3	E	133	G
3	E	136	A
3	E	137	C
3	E	138	U
3	E	139	C
3	E	148	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	136	A
3	E	137	C

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

1 non-standard protein/DNA/RNA residue is 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	GDP	E	99	3	30,30,30	0.86	0	44,47,47	4.87	8 (18%)

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	GDP	E	99	3	-	0/16/32/32	0/1/3/3

There are no bond length outliers.



All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	99	GDP	C6-C5-N7	-30.52	130.03	134.14
3	E	99	GDP	O3B-PB-O3A	-5.19	80.52	105.14
3	E	99	GDP	O3B-PB-O1B	-4.24	96.58	110.44
3	E	99	GDP	O2B-PB-O1B	3.47	121.78	110.44
3	E	99	GDP	C6-N1-C2	3.16	125.04	119.51
3	E	99	GDP	O2B-PB-O3A	2.80	118.44	105.14
3	E	99	GDP	O3B-PB-O2B	-2.64	97.33	107.61
3	E	99	GDP	C2-N3-C4	-2.28	111.89	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
4	SO4	A	1076	-	4,4,4	0.61	0	6,6,6	0.16	0
4	SO4	B	1002	-	4,4,4	0.62	0	6,6,6	0.17	0
4	SO4	E	1149	-	4,4,4	0.50	0	6,6,6	0.23	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	SO4	A	1076	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1149	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.