



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2016 – 10:27 AM EDT

PDB ID : 4O7U  
Title : Etherocomplex of Enterococcus faecalis thymidylate synthase with 5-hydroxy methylene-6-hydrofolic acid and the phtalimidic inhibitor SS7  
Authors : Mangani, S.; Pozzi, C.  
Deposited on : 2013-12-26  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

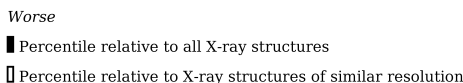
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

i

## X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
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Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

Mol	Chain	Length	Quality of chain
1	A	315	<p>4% 77% 15% 8%</p>
1	B	315	<p>89% 11%</p>
1	C	315	<p>2% 70% 16% 14%</p>
1	D	315	<p>85% 14%</p>

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SS7	D	402	-	-	X	X

## 2 Entry composition [i](#)

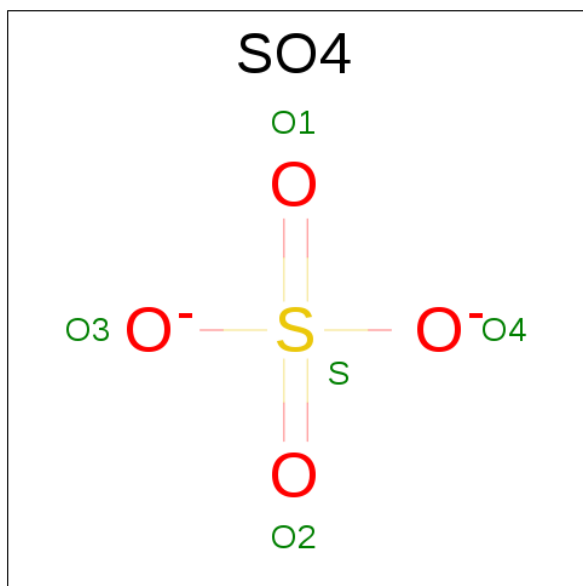
There are 6 unique types of molecules in this entry. The entry contains 10032 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2378	1533	394	441	10			
1	B	315	Total	C	N	O	S	0	0	0
			2569	1651	427	480	11			
1	C	272	Total	C	N	O	S	0	0	0
			2222	1436	370	407	9			
1	D	315	Total	C	N	O	S	0	0	0
			2569	1651	427	480	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



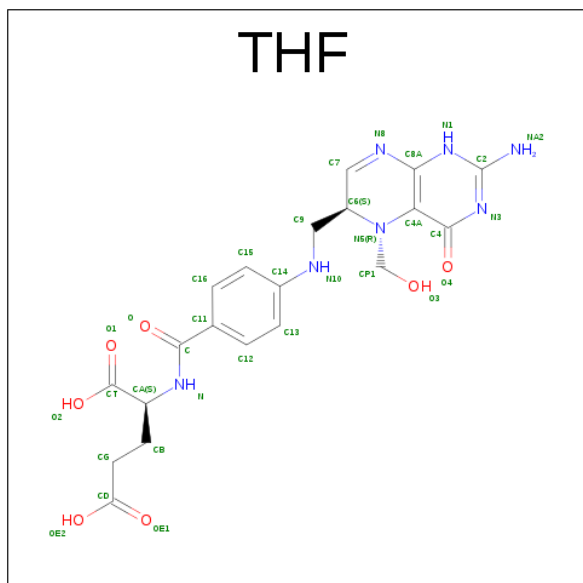
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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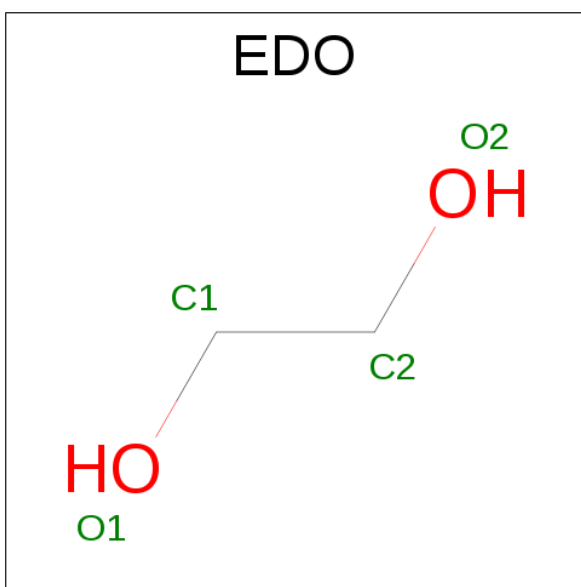
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5-HYDROXYMETHYLENE-6-HYDROFOLIC ACID (three-letter code: THF) (formula:  $C_{20}H_{23}N_7O_7$ ).



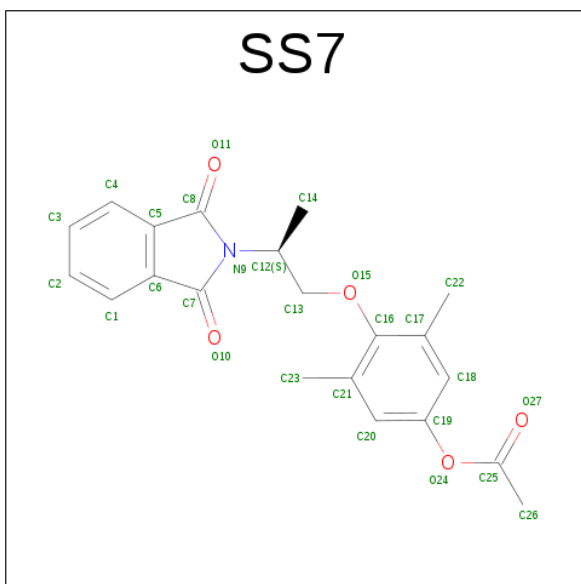
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 4-[(2S)-2-(1,3-DIOXO-1,3-DIHYDRO-2H-ISOINDOL-2-YL)PROPYL]OXY}-3,5-DIMETHYLPHENYL ACETATE (three-letter code: SS7) (formula: C<sub>21</sub>H<sub>21</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			27	21	1	5		

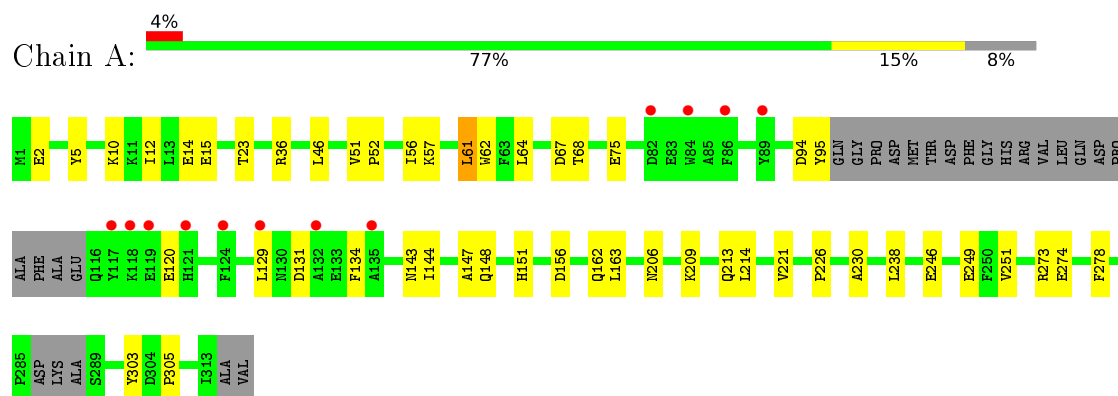
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total 38	O 38	0	0
6	B	69	Total 69	O 69	0	0
6	C	34	Total 34	O 34	0	0
6	D	64	Total 64	O 64	0	0

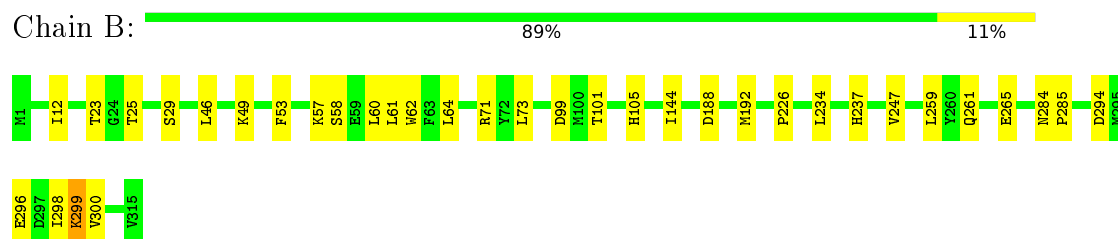
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

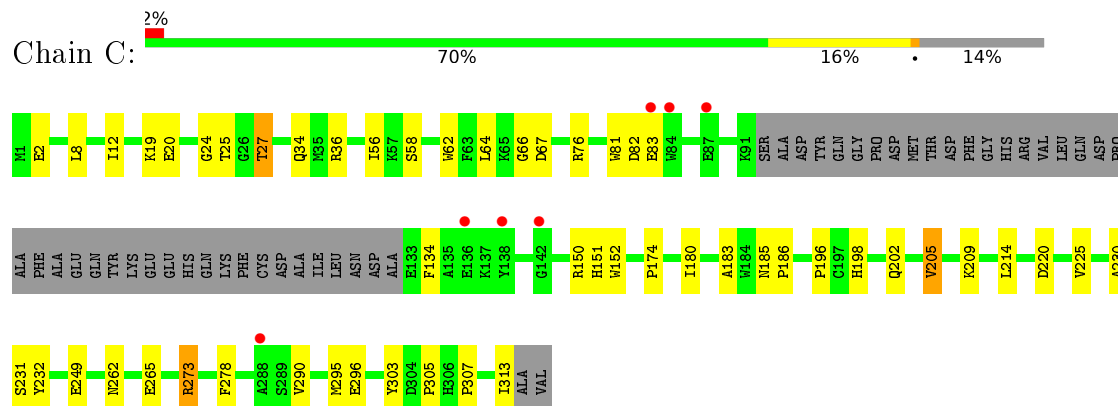
#### • Molecule 1: Thymidylate synthase

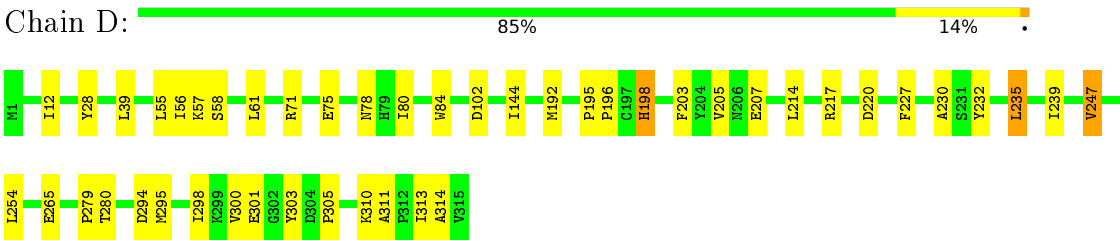


#### • Molecule 1: Thymidylate synthase



#### • Molecule 1: Thymidylate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.08Å 94.22Å 96.82Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	55.67 – 2.40 55.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	76.1 (55.67-2.40) 76.1 (55.67-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.212 , 0.287 0.213 , 0.288	Depositor DCC
$R_{free}$ test set	1962 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: THF, SS7, SO4, EDO

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	0.42	0/2443	0.61	1/3308 (0.0%)
1	B	0.45	0/2641	0.64	0/3579
1	C	0.42	0/2284	0.61	0/3095
1	D	0.45	0/2641	0.64	0/3579
All	All	0.44	0/10009	0.63	1/13561 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2378	0	2287	21	0
1	B	2569	0	2463	17	0
1	C	2222	0	2153	27	0
1	D	2569	0	2463	26	0
2	A	10	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
3	B	34	0	21	6	0
4	C	4	0	6	1	0
4	D	4	0	6	0	0
5	D	27	0	21	14	0
6	A	38	0	0	0	0
6	B	69	0	0	1	0
6	C	34	0	0	0	0
6	D	64	0	0	0	0
All	All	10032	0	9420	102	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 5.

All (102) 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)
5:D:402:SS7:H9	5:D:402:SS7:H12	1.45	0.97
5:D:402:SS7:C22	5:D:402:SS7:H9	1.95	0.95
1:C:174:PRO:HB2	1:C:205:VAL:HG11	1.56	0.86
1:B:46:LEU:HD22	1:B:226:PRO:HB3	1.57	0.86
3:B:401:THF:HCP1	3:B:401:THF:HN0	1.40	0.83
1:D:78:ASN:OD1	1:D:80:ILE:HG12	1.82	0.80
1:D:12:ILE:HD11	1:D:28:TYR:O	1.81	0.79
1:D:84:TRP:CZ2	5:D:402:SS7:H1	2.21	0.75
3:B:401:THF:O4	3:B:401:THF:HCP2	1.89	0.71
1:B:25:THR:O	1:B:261:GLN:NE2	2.27	0.68
1:B:296:GLU:OE1	1:B:299:LYS:NZ	2.26	0.67
3:B:401:THF:HCP1	3:B:401:THF:N10	2.09	0.67
1:C:174:PRO:CB	1:C:205:VAL:HG11	2.26	0.65
1:C:180:ILE:HD13	1:C:202:GLN:HB2	1.80	0.64
1:B:12:ILE:HG21	1:B:259:LEU:HB2	1.80	0.64
1:C:19:LYS:NZ	1:D:205:VAL:O	2.31	0.63
1:D:314:ALA:O	5:D:402:SS7:H2	1.99	0.62
1:A:57:LYS:O	1:A:61:LEU:HB2	2.01	0.61
1:A:64:LEU:CD2	1:A:163:LEU:HD21	2.33	0.59
1:A:148:GLN:O	1:A:162:GLN:NE2	2.36	0.59
1:C:174:PRO:HB2	1:C:205:VAL:CG1	2.30	0.59
1:C:198:HIS:HB3	1:C:214:LEU:HD11	1.84	0.59
5:D:402:SS7:C22	5:D:402:SS7:C13	2.78	0.58
1:A:10:LYS:O	1:A:14:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:HG3	1:A:129:LEU:HD11	1.85	0.57
1:B:23:THR:O	1:B:105:HIS:HE1	1.87	0.57
1:A:95:TYR:HE1	1:A:120:GLU:HG2	1.70	0.56
1:D:220:ASP:OD2	5:D:402:SS7:H4	2.06	0.56
1:C:56:ILE:HD13	1:C:230:ALA:HB3	1.90	0.54
3:B:401:THF:CP1	3:B:401:THF:N10	2.68	0.51
1:D:195:PRO:HG2	1:D:217:ARG:NH2	2.25	0.50
1:B:46:LEU:CD2	1:B:226:PRO:HB3	2.37	0.50
1:D:57:LYS:HD2	1:D:298:ILE:HB	1.93	0.50
1:A:2:GLU:HB2	1:A:278:PHE:CZ	2.47	0.50
1:C:8:LEU:O	1:C:12:ILE:HG13	2.12	0.49
1:D:227:PHE:CD2	5:D:402:SS7:H14	2.47	0.49
5:D:402:SS7:H18	5:D:402:SS7:C26	2.42	0.49
1:C:2:GLU:HB2	1:C:278:PHE:CZ	2.48	0.49
1:A:68:THR:HG21	1:A:147:ALA:HB2	1.94	0.48
1:C:62:TRP:CD1	1:C:67:ASP:HB3	2.48	0.47
1:A:64:LEU:HD22	1:A:163:LEU:HD21	1.95	0.47
1:C:220:ASP:O	1:C:225:VAL:HG23	2.14	0.47
1:B:265:GLU:OE1	1:D:265:GLU:OE1	2.32	0.47
1:C:152:TRP:CH2	1:C:185:ASN:HB2	2.49	0.47
1:C:56:ILE:HG23	1:C:231:SER:HB3	1.95	0.47
1:A:303:TYR:CZ	1:A:305:PRO:HG3	2.49	0.47
1:D:220:ASP:CB	5:D:402:SS7:H4	2.45	0.47
1:C:34:GLN:O	4:C:402:EDO:H12	2.15	0.47
1:A:131:ASP:HB3	1:A:134:PHE:HB3	1.97	0.46
1:D:198:HIS:HB2	1:D:214:LEU:HD11	1.96	0.46
1:B:234:LEU:HD11	1:B:298:ILE:HD13	1.98	0.46
1:C:58:SER:HA	1:C:295:MET:CE	2.46	0.46
1:D:203:PHE:CZ	1:D:239:ILE:HD12	2.51	0.46
1:A:51:VAL:HA	1:A:52:PRO:HD2	1.83	0.45
1:B:188:ASP:O	1:B:192:MET:HG3	2.16	0.45
1:C:313:ILE:HD12	1:C:313:ILE:H	1.81	0.45
1:C:20:GLU:OE2	1:C:24:GLY:HA2	2.17	0.45
1:A:62:TRP:CD1	1:A:67:ASP:HB3	2.52	0.45
1:B:23:THR:O	1:B:105:HIS:CE1	2.66	0.45
1:C:19:LYS:HB2	1:C:27:THR:HG22	1.99	0.45
1:A:36:ARG:HH21	1:A:249:GLU:CD	2.19	0.45
3:B:401:THF:CP1	3:B:401:THF:HN0	2.16	0.45
1:D:313:ILE:HG12	5:D:402:SS7:H15	2.00	0.44
1:A:213:GLN:HA	1:A:251:VAL:O	2.18	0.44
1:B:284:ASN:HA	1:B:285:PRO:HD2	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HG2	1:A:246:GLU:HB2	2.00	0.44
1:D:214:LEU:HD22	1:D:232:TYR:CD2	2.53	0.44
1:D:235:LEU:O	1:D:239:ILE:HG13	2.18	0.43
1:A:46:LEU:HD22	1:A:226:PRO:HB3	2.00	0.43
1:C:303:TYR:CZ	1:C:305:PRO:HG3	2.53	0.43
5:D:402:SS7:H18	5:D:402:SS7:H21	1.99	0.43
1:B:60:LEU:O	1:B:64:LEU:HG	2.17	0.43
1:C:36:ARG:NE	1:C:249:GLU:OE2	2.40	0.43
1:D:279:PRO:HB2	1:D:300:VAL:HG13	2.00	0.43
1:B:99:ASP:OD1	1:B:101:THR:HG23	2.18	0.43
1:D:84:TRP:HZ2	5:D:402:SS7:H1	1.75	0.43
1:C:273:ARG:NH2	1:C:307:PRO:O	2.52	0.43
1:D:192:MET:SD	1:D:196:PRO:HD3	2.59	0.43
1:C:209:LYS:HE3	1:C:209:LYS:HB2	1.90	0.43
1:C:64:LEU:HA	1:C:64:LEU:HD23	1.74	0.43
1:D:56:ILE:HD13	1:D:230:ALA:HB3	2.00	0.43
1:A:5:TYR:CE2	1:A:46:LEU:HD21	2.54	0.42
1:A:303:TYR:CE2	1:A:305:PRO:HG3	2.54	0.42
1:B:49:LYS:HD2	6:B:503:HOH:O	2.19	0.42
1:B:62:TRP:CZ3	1:B:73:LEU:HD11	2.54	0.42
1:D:303:TYR:CE2	1:D:305:PRO:HG3	2.54	0.42
1:B:237:HIS:CD2	1:B:247:VAL:HG11	2.55	0.42
1:C:185:ASN:HA	1:C:186:PRO:HD3	1.90	0.41
1:C:214:LEU:HD13	1:C:232:TYR:CE2	2.55	0.41
1:D:198:HIS:CD2	1:D:198:HIS:H	2.37	0.41
1:D:39:LEU:HB2	1:D:247:VAL:HG13	2.02	0.41
1:A:12:ILE:HD11	1:A:221:VAL:HG21	2.01	0.41
1:C:183:ALA:O	1:C:196:PRO:HG3	2.20	0.41
3:B:401:THF:CP1	3:B:401:THF:O4	2.66	0.41
5:D:402:SS7:H9	5:D:402:SS7:H13	1.94	0.41
1:D:71:ARG:O	1:D:75:GLU:HG3	2.22	0.40
1:C:66:GLY:HA3	1:C:150:ARG:HG3	2.03	0.40
1:D:58:SER:HB3	1:D:295:MET:SD	2.61	0.40
1:B:53:PHE:O	1:B:57:LYS:HG2	2.21	0.40
5:D:402:SS7:H17	5:D:402:SS7:C5	2.51	0.40
1:A:56:ILE:HD13	1:A:230:ALA:HB3	2.03	0.40
1:D:310:LYS:HD2	1:D:311:ALA:H	1.87	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	284/315 (90%)	270 (95%)	14 (5%)	0	100	100
1	B	313/315 (99%)	304 (97%)	8 (3%)	1 (0%)	46	63
1	C	268/315 (85%)	253 (94%)	15 (6%)	0	100	100
1	D	313/315 (99%)	303 (97%)	9 (3%)	1 (0%)	46	63
All	All	1178/1260 (94%)	1130 (96%)	46 (4%)	2 (0%)	52	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	144	ILE
1	B	144	ILE

### 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	254/273 (93%)	242 (95%)	12 (5%)	32	50
1	B	273/273 (100%)	266 (97%)	7 (3%)	54	74
1	C	237/273 (87%)	223 (94%)	14 (6%)	24	38
1	D	273/273 (100%)	262 (96%)	11 (4%)	38	58
All	All	1037/1092 (95%)	993 (96%)	44 (4%)	36	56

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	23	THR
1	A	61	LEU
1	A	94	ASP
1	A	143	ASN
1	A	144	ILE
1	A	151	HIS
1	A	156	ASP
1	A	206	ASN
1	A	238	LEU
1	A	273	ARG
1	A	274	GLU
1	B	29	SER
1	B	58	SER
1	B	61	LEU
1	B	71	ARG
1	B	294	ASP
1	B	299	LYS
1	B	300	VAL
1	C	25	THR
1	C	27	THR
1	C	76	ARG
1	C	81	TRP
1	C	82	ASP
1	C	83	GLU
1	C	134	PHE
1	C	151	HIS
1	C	205	VAL
1	C	262	ASN
1	C	265	GLU
1	C	273	ARG
1	C	290	VAL
1	C	296	GLU
1	D	55	LEU
1	D	61	LEU
1	D	102	ASP
1	D	198	HIS
1	D	207	GLU
1	D	235	LEU
1	D	247	VAL
1	D	254	LEU
1	D	280	THR
1	D	294	ASP

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Mol	Chain	Res	Type
1	D	301	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	D	34	GLN
1	D	213	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	A	401	-	4,4,4	0.27	0	6,6,6	0.56	0
2	SO4	A	402	-	4,4,4	0.40	0	6,6,6	0.25	0
3	THF	B	401	-	26,36,36	2.00	3 (11%)	24,50,50	1.89	6 (25%)
2	SO4	C	401	-	4,4,4	0.36	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	402	-	3,3,3	0.64	0	2,2,2	0.08	0
2	SO4	D	401	-	4,4,4	0.41	0	6,6,6	0.51	0
5	SS7	D	402	-	28,29,29	2.88	6 (21%)	40,42,42	3.60	19 (47%)
4	EDO	D	403	-	3,3,3	0.44	0	2,2,2	0.46	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
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
3	THF	B	401	-	-	0/14/37/37	0/3/3/3
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
4	EDO	C	402	-	-	0/1/1/1	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
5	SS7	D	402	-	-	0/13/29/29	0/3/3/3
4	EDO	D	403	-	-	0/1/1/1	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	402	SS7	C5-C8	-5.90	1.39	1.48
5	D	402	SS7	C8-N9	-3.65	1.33	1.40
5	D	402	SS7	C7-N9	-2.55	1.35	1.40
5	D	402	SS7	O11-C8	2.45	1.27	1.22
5	D	402	SS7	O24-C25	3.11	1.46	1.36
3	B	401	THF	C4-C4A	4.50	1.47	1.41
3	B	401	THF	C4A-C8A	5.52	1.48	1.41
3	B	401	THF	C7-N8	6.20	1.34	1.27
5	D	402	SS7	O10-C7	12.19	1.47	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	402	SS7	C7-N9-C8	-9.86	102.47	111.56
5	D	402	SS7	C5-C6-C7	-5.72	103.29	108.28
5	D	402	SS7	O10-C7-C6	-4.90	119.06	128.70
5	D	402	SS7	O24-C25-O27	-3.52	114.37	122.36
3	B	401	THF	C4A-C4-N3	-3.33	118.44	123.39
5	D	402	SS7	O11-C8-C5	-2.96	122.87	128.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	402	SS7	C6-C5-C8	-2.93	105.73	108.28
3	B	401	THF	O-C-C11	-2.80	116.16	120.95
5	D	402	SS7	O11-C8-N9	-2.72	121.41	124.94
3	B	401	THF	CT-CA-N	2.05	117.02	112.93
5	D	402	SS7	C13-O15-C16	2.12	121.98	114.24
3	B	401	THF	C4-C4A-C8A	2.30	116.24	114.45
5	D	402	SS7	C1-C6-C7	2.47	133.52	129.64
5	D	402	SS7	O10-C7-N9	2.47	128.16	124.94
5	D	402	SS7	C12-N9-C7	2.61	132.07	123.90
5	D	402	SS7	C4-C5-C8	2.78	134.00	129.64
5	D	402	SS7	O15-C16-C17	2.79	123.33	118.94
5	D	402	SS7	C20-C21-C16	3.32	122.67	117.83
3	B	401	THF	C11-C-N	3.44	123.00	116.98
5	D	402	SS7	O15-C13-C12	3.51	115.17	107.94
5	D	402	SS7	C19-O24-C25	4.33	130.55	118.73
3	B	401	THF	C4-N3-C2	5.03	121.78	115.88
5	D	402	SS7	O24-C25-C26	5.27	122.43	110.91
5	D	402	SS7	C6-C7-N9	7.97	112.79	105.90
5	D	402	SS7	C5-C8-N9	11.36	115.72	105.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	THF	6	0
4	C	402	EDO	1	0
5	D	402	SS7	14	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	290/315 (92%)	0.10	12 (4%) 41 42	7, 15, 56, 77	0
1	B	315/315 (100%)	-0.20	0 100 100	5, 9, 21, 29	0
1	C	272/315 (86%)	0.05	7 (2%) 59 58	6, 14, 49, 67	0
1	D	315/315 (100%)	-0.21	0 100 100	4, 9, 28, 39	0
All	All	1192/1260 (94%)	-0.07	19 (1%) 74 74	4, 11, 44, 77	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	TYR	4.1
1	A	84	TRP	4.0
1	A	132	ALA	3.9
1	C	142	GLY	3.8
1	A	121	HIS	3.1
1	C	288	ALA	2.9
1	A	129	LEU	2.9
1	C	84	TRP	2.8
1	A	135	ALA	2.8
1	A	89	TYR	2.7
1	A	82	ASP	2.6
1	A	119	GLU	2.4
1	A	118	LYS	2.3
1	A	86	PHE	2.3
1	C	87	GLU	2.1
1	A	124	PHE	2.1
1	C	136	GLU	2.1
1	C	83	GLU	2.1
1	C	138	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SS7	D	402	27/27	0.90	0.18	2.24	10,11,13,13	0
4	EDO	D	403	4/4	0.97	0.17	1.51	17,17,17,18	0
3	THF	B	401	34/34	0.90	0.15	0.42	10,10,11,12	0
2	SO4	C	401	5/5	0.97	0.18	0.41	30,30,31,32	0
2	SO4	D	401	5/5	0.98	0.15	0.19	10,10,10,10	0
2	SO4	A	401	5/5	0.96	0.13	-0.01	13,13,14,14	0
2	SO4	A	402	5/5	0.92	0.14	-0.33	34,35,36,36	0
4	EDO	C	402	4/4	0.91	0.21	-	7,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.