Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:46 PM GMT

PDB ID	:	3UWL
Title	:	Crystal structure of Enteroccocus faecalis thymidylate synthase (EfTS) in complex with 5-formyl tetrahydrofolate
Authors	:	Pozzi, C.; Catalano, A.; Cortesi, D.; Luciani, R.; Ferrari, S.; Fritz, T.; Costi, M.P.; Mangani, S.
Deposited on	:	2011-12-02
Resolution	:	2.07 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

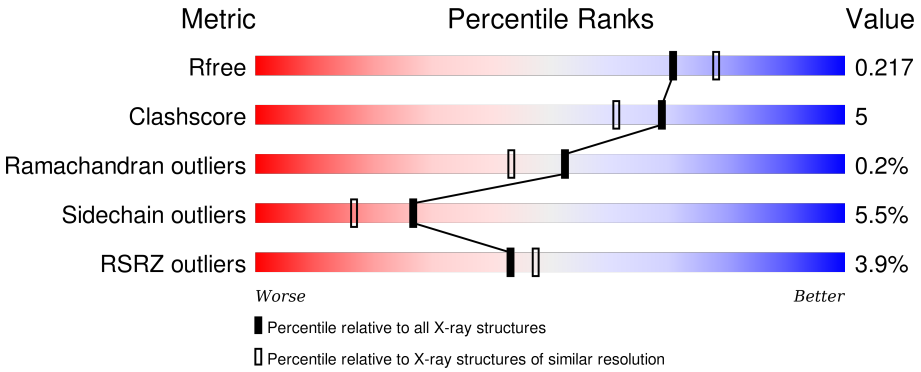
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	315	6%, 80%, 10%, 7%
1	C	315	9%, 78%, 10%, 10%
2	B	315	91%, 9%
2	D	315	90%, 9%

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
5	EDO	B	322	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10751 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.

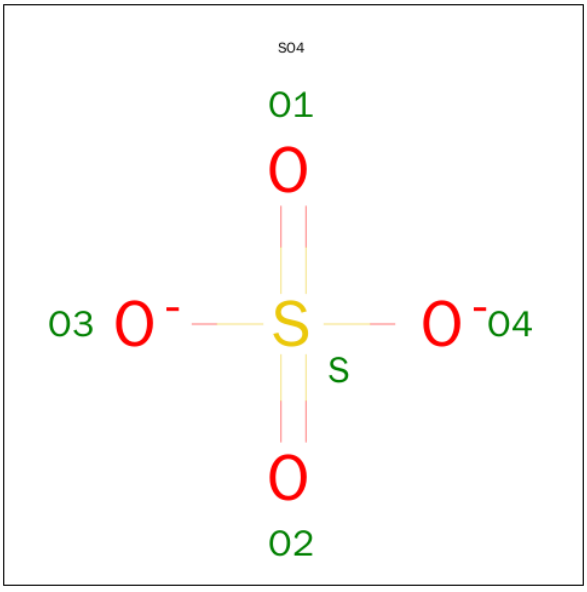
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2380	1532	396	442	10			
1	C	282	Total	C	N	O	S	0	0	0
			2302	1486	382	424	10			

- Molecule 2 is a protein called Thymidylate synthase.

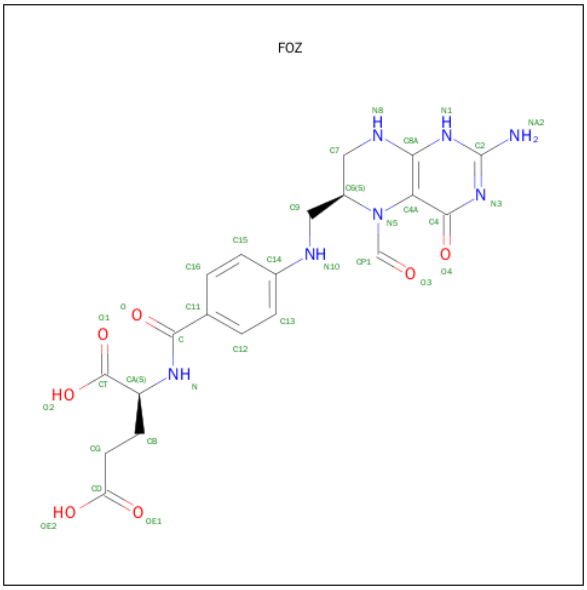
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	0	0
			2573	1653	427	481	12			
2	D	315	Total	C	N	O	S	0	0	0
			2567	1651	427	477	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



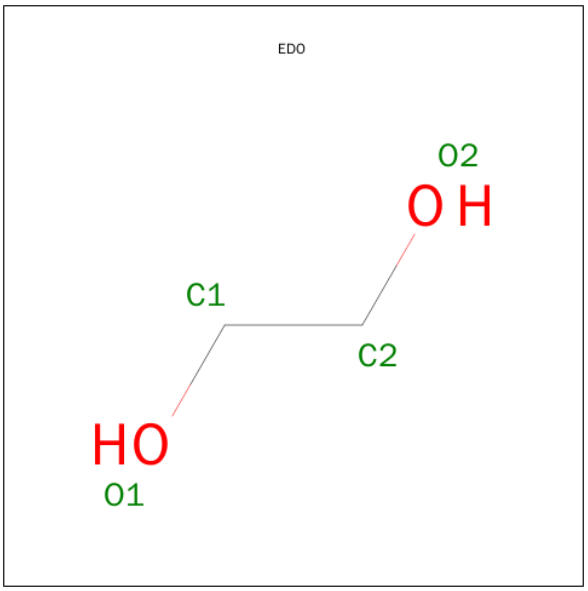
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is N-[4-({[(6S)-2-AMINO-5-FORMYL-4-OXO-1,4,5,6,7,8-HEXAHYDROPTERIDIN-6-YL]METHYL}AMINO)BENZOYL]-L-GLUTAMIC ACID (three-letter code: FOZ) (formula: $C_{20}H_{23}N_7O_7$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

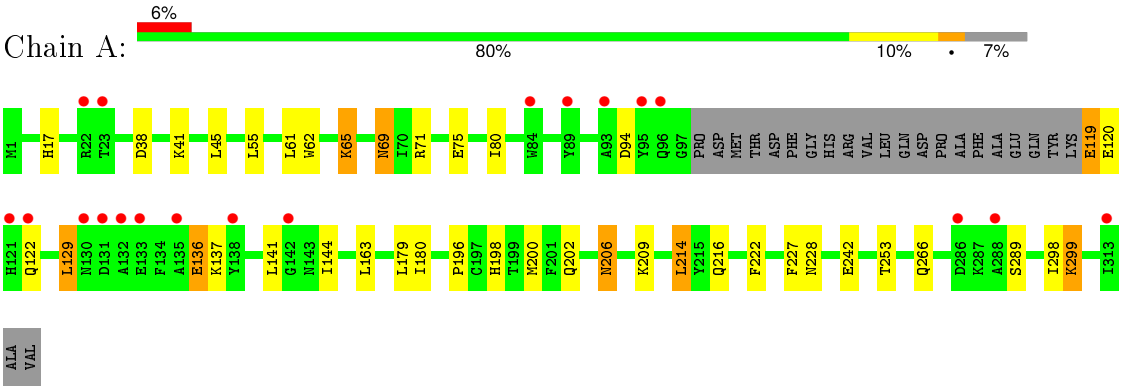
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	162	Total O 162 162	0	0
6	B	244	Total O 244 244	0	0
6	C	130	Total O 130 130	0	0
6	D	263	Total O 263 263	0	0

3 Residue-property plots

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.

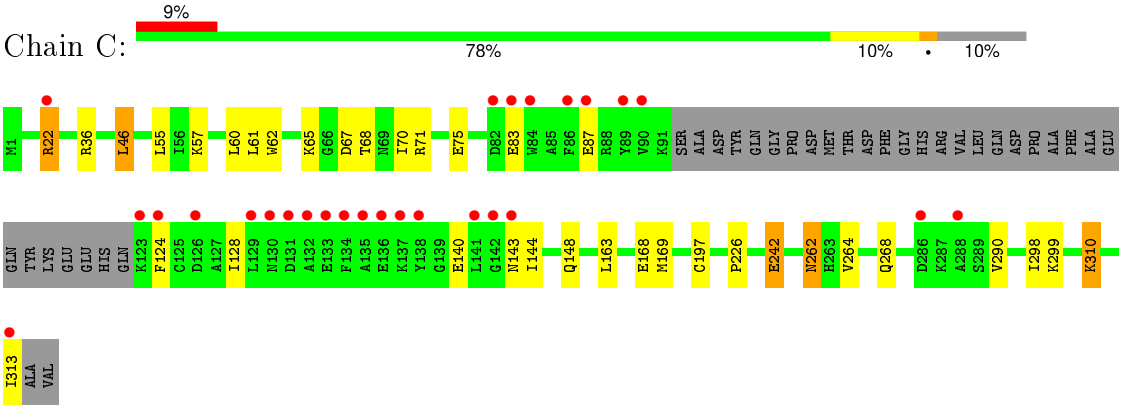
- Molecule 1: Thymidylate synthase

Chain A:



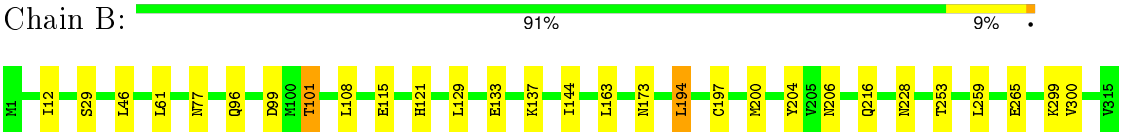
- Molecule 1: Thymidylate synthase

Chain C:



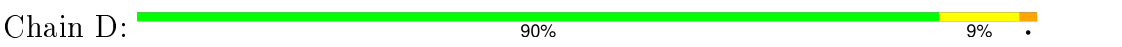
- Molecule 2: Thymidylate synthase

Chain B:



- Molecule 2: Thymidylate synthase

Chain D:




M1
L30
I56
L61
K65
R71
N77
D82
D99
M100
T101
E119
E120
H121
L129
K137
Y138
I144
Y145
H151
K155
L163
N173
S176
L179
I180
V181
C197
H198
N206
L214
Y215
Q216
N228
I229
A230
S231
Y232
E265
V315

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.94Å 94.25Å 96.19Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	33.49 – 2.07 33.49 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.2 (33.49-2.07) 96.2 (33.49-2.07)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.160 , 0.217 0.162 , 0.217	Depositor DCC
R_{free} test set	3757 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 75020 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10751	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CME, SO4, FOZ, 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	0.74	0/2445	0.73	0/3312
1	C	0.72	1/2365 (0.0%)	0.70	0/3204
2	B	0.78	0/2634	0.75	1/3568 (0.0%)
2	D	0.78	0/2628	0.76	2/3560 (0.1%)
All	All	0.75	1/10072 (0.0%)	0.74	3/13644 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	CYS	CB-SG	5.46	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	194	LEU	CA-CB-CG	5.81	128.67	115.30
2	D	30	LEU	CA-CB-CG	5.47	127.88	115.30
2	D	71	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	2380	0	2289	28	0
1	C	2302	0	2230	27	0
2	B	2573	0	2467	15	0
2	D	2567	0	2463	23	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	B	34	0	21	2	0
4	D	34	0	21	0	0
5	B	16	0	24	0	0
5	C	8	0	12	2	0
5	D	8	0	12	0	0
6	A	162	0	0	4	0
6	B	244	0	0	5	0
6	C	130	0	0	7	0
6	D	263	0	0	5	0
All	All	10751	0	9539	90	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 (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LYS:H	1:C:310:LYS:HD3	1.17	1.07
2:D:206:ASN:HB2	6:D:796:HOH:O	1.54	1.05
1:C:65:LYS:HB3	6:C:440:HOH:O	1.62	0.99
1:C:242:GLU:HG3	1:C:290:VAL:HG22	1.52	0.90
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.36	0.89
1:A:299:LYS:HE3	6:A:384:HOH:O	1.76	0.85
1:C:262:ASN:HD22	1:C:262:ASN:H	1.28	0.81
1:A:206:ASN:HB2	6:B:595:HOH:O	1.82	0.80
1:A:227:PHE:HB3	6:A:716:HOH:O	1.84	0.75
1:C:310:LYS:H	1:C:310:LYS:CD	1.93	0.75
2:D:99:ASP:OD1	2:D:101:THR:HG23	1.86	0.75
1:A:65:LYS:HD3	6:A:793:HOH:O	1.85	0.75
1:C:169:MET:HG2	6:C:672:HOH:O	1.87	0.75
2:B:99:ASP:OD1	2:B:101:THR:CG2	2.37	0.72
1:C:36:ARG:HG3	5:C:318:EDO:H12	1.73	0.69
2:B:99:ASP:OD1	2:B:101:THR:HG22	1.97	0.65
2:D:145:TYR:CZ	2:D:198:HIS:NE2	2.65	0.65
1:C:22:ARG:HH11	1:C:22:ARG:CG	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:TYR:CZ	2:D:198:HIS:CE1	2.86	0.63
2:B:265:GLU:HG3	2:D:265:GLU:HG3	1.80	0.63
1:A:298:ILE:O	1:A:299:LYS:HD2	1.98	0.63
2:D:216:GLN:HE22	2:D:228:ASN:ND2	1.96	0.62
1:C:46:LEU:HD22	1:C:226:PRO:HB3	1.80	0.61
2:B:77:ASN:HB3	6:B:772:HOH:O	2.00	0.61
1:A:69:ASN:HD22	1:A:71:ARG:H	1.48	0.61
2:B:99:ASP:OD1	2:B:101:THR:HG23	2.00	0.61
1:A:62:TRP:HH2	1:A:141:LEU:HD12	1.67	0.59
1:A:298:ILE:C	1:A:299:LYS:HD2	2.23	0.59
2:B:115:GLU:HG3	6:B:550:HOH:O	2.02	0.58
1:C:143:ASN:HB2	6:C:753:HOH:O	2.03	0.58
1:C:65:LYS:CG	1:C:67:ASP:HB2	2.34	0.57
1:A:242:GLU:OE2	1:A:289:SER:HA	2.04	0.57
2:D:145:TYR:HE1	2:D:198:HIS:O	1.88	0.57
1:A:65:LYS:HB3	1:A:65:LYS:NZ	2.19	0.56
1:A:75:GLU:HG3	1:A:129:LEU:HD11	1.87	0.56
2:D:145:TYR:CE1	2:D:198:HIS:CE1	2.93	0.56
1:A:198:HIS:HB3	1:A:214:LEU:HD21	1.86	0.56
4:B:316:FOZ:CP1	6:B:365:HOH:O	2.53	0.55
1:A:38:ASP:HB3	1:A:41:LYS:HD2	1.89	0.55
2:D:198:HIS:CD2	2:D:198:HIS:H	2.23	0.54
2:D:77:ASN:ND2	6:D:441:HOH:O	2.40	0.53
2:D:56:ILE:HD13	2:D:230:ALA:HB3	1.90	0.53
2:D:197:CME:O	2:D:216:GLN:HG3	2.08	0.53
1:C:310:LYS:HE3	6:C:373:HOH:O	2.09	0.53
1:A:180:ILE:HD13	1:A:202:GLN:HB2	1.90	0.53
2:D:151:HIS:HE1	6:D:558:HOH:O	1.93	0.52
2:B:216:GLN:HE22	2:B:228:ASN:ND2	2.06	0.52
1:A:222:PHE:CZ	1:A:266:GLN:HB3	2.45	0.52
2:D:145:TYR:OH	2:D:198:HIS:CD2	2.63	0.52
1:C:310:LYS:HD3	1:C:310:LYS:N	2.03	0.52
2:D:173:ASN:HD22	2:D:176:SER:HB2	1.75	0.51
2:B:197:CME:SD	4:B:316:FOZ:HP1	2.50	0.51
2:D:121:HIS:HD2	6:D:601:HOH:O	1.93	0.51
1:C:262:ASN:H	1:C:262:ASN:ND2	2.03	0.50
1:A:144:ILE:CD1	6:A:331:HOH:O	2.59	0.49
2:B:12:ILE:HG21	2:B:259:LEU:HB2	1.94	0.49
1:C:62:TRP:CD1	1:C:67:ASP:HB3	2.48	0.49
5:C:318:EDO:H11	6:C:795:HOH:O	2.12	0.49
1:C:124:PHE:O	1:C:128:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ASN:N	1:C:262:ASN:HD22	2.06	0.47
1:A:216:GLN:HE22	1:A:228:ASN:ND2	2.11	0.47
2:D:99:ASP:OD1	2:D:101:THR:CG2	2.60	0.46
1:A:65:LYS:HB3	1:A:65:LYS:HZ1	1.80	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HB2	1.64	0.46
1:A:75:GLU:CG	1:A:129:LEU:HD11	2.44	0.46
1:C:68:THR:HG23	1:C:140:GLU:OE1	2.16	0.46
1:C:242:GLU:HG3	1:C:290:VAL:CG2	2.36	0.46
2:D:71:ARG:NH2	2:D:129:LEU:O	2.50	0.45
1:C:264:VAL:O	1:C:268:GLN:HG3	2.17	0.45
2:B:137:LYS:HB2	2:B:137:LYS:HE3	1.56	0.45
1:C:310:LYS:HG3	6:C:769:HOH:O	2.17	0.45
1:A:200:MET:HE2	2:B:200:MET:HE1	1.99	0.44
2:B:121:HIS:HD2	6:B:625:HOH:O	2.00	0.44
1:A:119:GLU:HG3	1:A:120:GLU:N	2.33	0.43
1:C:22:ARG:HD2	6:C:495:HOH:O	2.17	0.43
1:C:65:LYS:HG3	1:C:67:ASP:HB2	2.00	0.42
1:A:200:MET:HE2	1:A:200:MET:HB3	1.97	0.42
2:D:214:LEU:HD22	2:D:232:TYR:CD2	2.54	0.42
2:D:155:LYS:HE2	6:D:560:HOH:O	2.20	0.42
1:C:57:LYS:NZ	1:C:298:ILE:O	2.51	0.41
1:A:136:GLU:HG2	1:A:136:GLU:H	1.60	0.41
1:A:200:MET:HE3	2:B:200:MET:HE3	2.02	0.41
1:A:17:HIS:HD2	2:B:204:TYR:OH	2.02	0.41
2:D:137:LYS:HG2	2:D:138:TYR:CE1	2.55	0.41
1:C:71:ARG:O	1:C:75:GLU:HG3	2.21	0.41
1:A:69:ASN:ND2	1:A:71:ARG:H	2.17	0.41
1:A:253:THR:HG21	2:B:253:THR:HG21	2.02	0.41
2:D:82:ASP:OD1	2:D:121:HIS:CE1	2.74	0.40
2:D:163:LEU:HD23	2:D:181:VAL:HG21	2.02	0.40
1:C:22:ARG:NH1	1:C:22:ARG:CG	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	288/315 (91%)	279 (97%)	9 (3%)	0	100 100
1	C	278/315 (88%)	268 (96%)	10 (4%)	0	100 100
2	B	312/315 (99%)	304 (97%)	7 (2%)	1 (0%)	46 36
2	D	312/315 (99%)	305 (98%)	6 (2%)	1 (0%)	46 36
All	All	1190/1260 (94%)	1156 (97%)	32 (3%)	2 (0%)	52 43

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	253/273 (93%)	235 (93%)	18 (7%)	18 9
1	C	246/273 (90%)	229 (93%)	17 (7%)	19 10
2	B	272/272 (100%)	258 (95%)	14 (5%)	29 19
2	D	270/272 (99%)	262 (97%)	8 (3%)	48 42
All	All	1041/1090 (96%)	984 (94%)	57 (6%)	27 17

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	55	LEU
1	A	61	LEU
1	A	65	LYS
1	A	69	ASN
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	94	ASP
1	A	119	GLU
1	A	122	GLN
1	A	129	LEU
1	A	136	GLU
1	A	137	LYS
1	A	163	LEU
1	A	179	LEU
1	A	196	PRO
1	A	206	ASN
1	A	214	LEU
1	A	299	LYS
2	B	29	SER
2	B	46	LEU
2	B	61	LEU
2	B	96	GLN
2	B	101	THR
2	B	108	LEU
2	B	129	LEU
2	B	133	GLU
2	B	163	LEU
2	B	173	ASN
2	B	194	LEU
2	B	206	ASN
2	B	299	LYS
2	B	300	VAL
1	C	22	ARG
1	C	46	LEU
1	C	55	LEU
1	C	60	LEU
1	C	61	LEU
1	C	70	ILE
1	C	83	GLU
1	C	87	GLU
1	C	144	ILE
1	C	148	GLN
1	C	163	LEU
1	C	168	GLU
1	C	242	GLU
1	C	262	ASN
1	C	299	LYS
1	C	310	LYS

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Mol	Chain	Res	Type
1	C	313	ILE
2	D	30	LEU
2	D	61	LEU
2	D	65	LYS
2	D	101	THR
2	D	119	GLU
2	D	129	LEU
2	D	163	LEU
2	D	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	69	ASN
1	A	121	HIS
1	A	130	ASN
1	A	148	GLN
1	A	151	HIS
1	A	228	ASN
1	A	261	GLN
2	B	121	HIS
2	B	228	ASN
2	B	270	GLN
1	C	17	HIS
1	C	148	GLN
1	C	261	GLN
1	C	262	ASN
1	C	270	GLN
2	D	77	ASN
2	D	121	HIS
2	D	151	HIS
2	D	173	ASN
2	D	228	ASN
2	D	268	GLN
2	D	270	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	CME	B	197	2	8,9,10	0.65	0	6,9,11	1.70	1 (16%)
2	CME	D	197	2	8,9,10	0.66	0	6,9,11	1.90	2 (33%)

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	CME	B	197	2	-	0/5/8/10	0/0/0/0
2	CME	D	197	2	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	197	CME	CE-SD-SG	2.39	115.94	103.56
2	D	197	CME	CB-SG-SD	2.87	109.55	103.95
2	B	197	CME	CB-SG-SD	3.32	110.41	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	197	CME	1	0
2	D	197	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	FOZ	B	316	-	27,36,36	1.13	2 (7%)	30,50,50	2.01	7 (23%)
3	SO4	B	317	-	4,4,4	0.49	0	6,6,6	0.13	0
3	SO4	B	318	-	4,4,4	0.50	0	6,6,6	0.79	0
3	SO4	B	319	-	4,4,4	0.30	0	6,6,6	0.13	0
5	EDO	B	320	-	3,3,3	0.50	0	2,2,2	0.46	0
5	EDO	B	321	-	3,3,3	0.68	0	2,2,2	0.25	0
5	EDO	B	322	-	3,3,3	0.60	0	2,2,2	0.18	0
5	EDO	B	323	-	3,3,3	0.48	0	2,2,2	0.71	0
3	SO4	C	317	-	4,4,4	0.49	0	6,6,6	0.43	0
5	EDO	C	318	-	3,3,3	0.47	0	2,2,2	0.49	0
5	EDO	C	319	-	3,3,3	0.41	0	2,2,2	0.61	0
4	FOZ	D	316	-	27,36,36	1.14	3 (11%)	30,50,50	1.84	7 (23%)
3	SO4	D	317	-	4,4,4	0.37	0	6,6,6	0.32	0
3	SO4	D	318	-	4,4,4	0.19	0	6,6,6	0.20	0
5	EDO	D	320	-	3,3,3	0.60	0	2,2,2	0.15	0
5	EDO	D	321	-	3,3,3	0.30	0	2,2,2	1.40	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	FOZ	B	316	-	-	0/18/37/37	0/2/3/3
3	SO4	B	317	-	-	0/0/0/0	0/0/0/0
3	SO4	B	318	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	319	-	-	0/0/0/0	0/0/0/0
5	EDO	B	320	-	-	0/1/1/1	0/0/0/0
5	EDO	B	321	-	-	0/1/1/1	0/0/0/0
5	EDO	B	322	-	-	0/1/1/1	0/0/0/0
5	EDO	B	323	-	-	0/1/1/1	0/0/0/0
3	SO4	C	317	-	-	0/0/0/0	0/0/0/0
5	EDO	C	318	-	-	0/1/1/1	0/0/0/0
5	EDO	C	319	-	-	0/1/1/1	0/0/0/0
4	FOZ	D	316	-	-	0/18/37/37	0/2/3/3
3	SO4	D	317	-	-	0/0/0/0	0/0/0/0
3	SO4	D	318	-	-	0/0/0/0	0/0/0/0
5	EDO	D	320	-	-	0/1/1/1	0/0/0/0
5	EDO	D	321	-	-	0/1/1/1	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	316	FOZ	C4-N3	2.09	1.37	1.33
4	D	316	FOZ	CP1-N5	2.11	1.41	1.36
4	B	316	FOZ	CP1-N5	2.55	1.41	1.36
4	B	316	FOZ	C4A-C8A	3.43	1.48	1.41
4	D	316	FOZ	C4A-C8A	3.55	1.48	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	316	FOZ	O3-CP1-N5	-4.80	117.00	124.21
4	D	316	FOZ	O3-CP1-N5	-4.39	117.62	124.21
4	B	316	FOZ	C4A-C4-N3	-3.94	117.40	123.46
4	D	316	FOZ	C4A-N5-C6	-3.72	113.34	119.81
4	B	316	FOZ	C4A-N5-C6	-3.43	113.84	119.81
4	D	316	FOZ	C4A-C4-N3	-3.00	118.84	123.46
4	D	316	FOZ	C11-C-N	2.25	120.94	116.93
4	B	316	FOZ	C11-C-N	2.54	121.45	116.93
4	D	316	FOZ	C4-C4A-C8A	2.81	116.67	114.43
4	B	316	FOZ	C2-N1-C8A	3.07	121.44	114.54
4	D	316	FOZ	C2-N1-C8A	3.46	122.32	114.54
4	D	316	FOZ	C4-N3-C2	3.49	120.79	115.94
4	B	316	FOZ	C4-C4A-C8A	3.60	117.30	114.43
4	B	316	FOZ	C4-N3-C2	4.24	121.83	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	316	FOZ	2	0
5	C	318	EDO	2	0

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

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	A	292/315 (92%)	-0.00	19 (6%) 22 24	5, 16, 56, 78	0
1	C	282/315 (89%)	0.12	27 (9%) 10 11	6, 17, 67, 83	0
2	B	314/315 (99%)	-0.47	0 100 100	5, 10, 23, 39	0
2	D	314/315 (99%)	-0.48	1 (0%) 94 95	5, 10, 23, 37	0
All	All	1202/1260 (95%)	-0.22	47 (3%) 43 47	5, 13, 45, 83	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	GLY	6.9
1	C	138	TYR	5.5
1	C	89	TYR	5.3
1	C	132	ALA	5.1
1	A	84	TRP	5.0
1	C	133	GLU	4.9
1	C	136	GLU	4.7
1	C	86	PHE	4.7
1	C	288	ALA	4.5
1	A	132	ALA	3.8
1	C	90	VAL	3.4
1	C	141	LEU	3.4
1	C	286	ASP	3.4
1	C	134	PHE	3.3
1	A	22	ARG	3.3
1	C	124	PHE	3.0
1	A	121	HIS	3.0
1	A	133	GLU	3.0
1	A	93	ALA	3.0
1	A	313	ILE	2.9
1	A	23	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	89	TYR	2.7
1	C	123	LYS	2.7
1	A	288	ALA	2.6
2	D	198	HIS	2.6
1	C	126	ASP	2.6
1	A	96	GLN	2.5
1	C	82	ASP	2.5
1	C	313	ILE	2.5
1	A	130	ASN	2.5
1	A	286	ASP	2.5
1	C	87	GLU	2.4
1	C	131	ASP	2.4
1	C	84	TRP	2.4
1	A	135	ALA	2.4
1	C	137	LYS	2.3
1	A	95	TYR	2.3
1	C	83	GLU	2.3
1	C	129	LEU	2.3
1	A	142	GLY	2.3
1	C	130	ASN	2.3
1	A	122	GLN	2.2
1	A	138	TYR	2.2
1	C	143	ASN	2.1
1	A	131	ASP	2.1
1	C	135	ALA	2.1
1	C	22	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	CME	B	197	10/11	0.94	0.12	-	11,14,23,31	0
2	CME	D	197	10/11	0.95	0.14	-	11,14,22,31	0

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^{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	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	B	322	4/4	0.79	0.18	4.21	27,27,28,28	0
5	EDO	B	323	4/4	0.96	0.10	1.77	16,19,19,19	0
5	EDO	B	320	4/4	0.97	0.11	1.19	18,20,21,26	0
5	EDO	D	320	4/4	0.94	0.11	1.10	20,21,22,24	0
4	FOZ	B	316	34/34	0.95	0.10	0.37	6,13,17,20	0
4	FOZ	D	316	34/34	0.94	0.11	0.20	11,15,19,24	0
5	EDO	C	319	4/4	0.98	0.10	0.10	23,24,25,26	0
3	SO4	B	318	5/5	0.98	0.10	-0.08	26,28,30,32	0
3	SO4	C	317	5/5	0.97	0.10	-0.70	33,34,37,37	0
3	SO4	B	317	5/5	0.99	0.08	-0.74	17,18,21,21	0
3	SO4	D	317	5/5	1.00	0.08	-1.02	15,15,16,18	0
5	EDO	D	321	4/4	0.90	0.13	-	20,22,22,23	0
5	EDO	C	318	4/4	0.89	0.19	-	21,29,29,31	0
3	SO4	B	319	5/5	0.97	0.20	-	46,47,48,48	0
5	EDO	B	321	4/4	0.65	0.21	-	31,32,34,36	0
3	SO4	D	318	5/5	0.97	0.20	-	46,47,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.