Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:55 PM GMT

PDB ID	:	1HVY
Title	:	Human thymidylate synthase complexed with dUMP and Raltitrexed, an antifolate drug, is in the closed conformation
Authors	:	Phan, J.; Koli, S.; Minor, W.; Dunlap, R.B.; Berger, S.H.; Lebioda, L.
Deposited on	:	2001-01-08
Resolution	:	1.90 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:

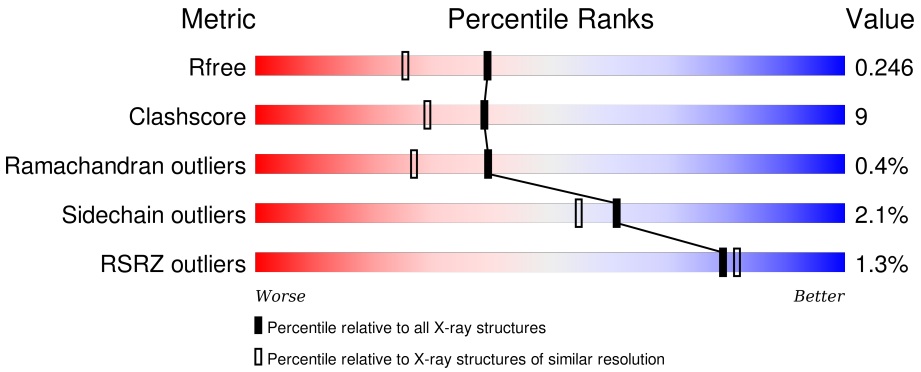
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	288	81% 19%
1	B	288	82% 18%
1	C	288	79% 20%
1	D	288	80% 17%

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
4	BME	A	1514	-	-	-	X
4	BME	C	1516	-	-	-	X
4	BME	D	1517	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10136 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.

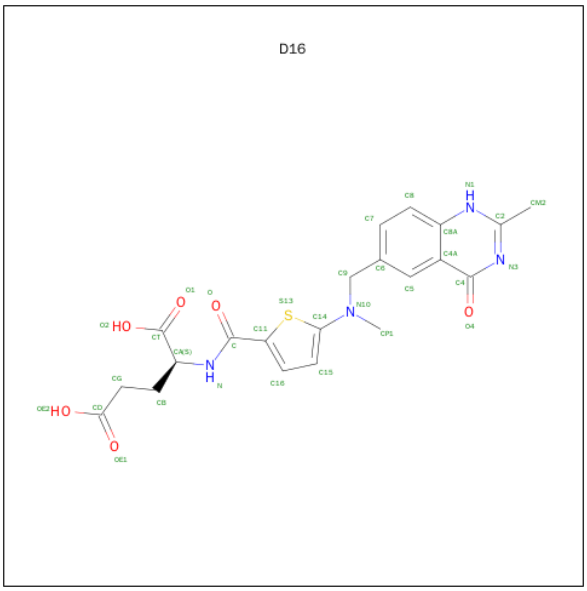
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			
1	B	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			
1	C	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			
1	D	288	Total	C	N	O	S	0	0	0
			2329	1488	405	422	14			

There are 4 discrepancies between the modelled and reference sequences:

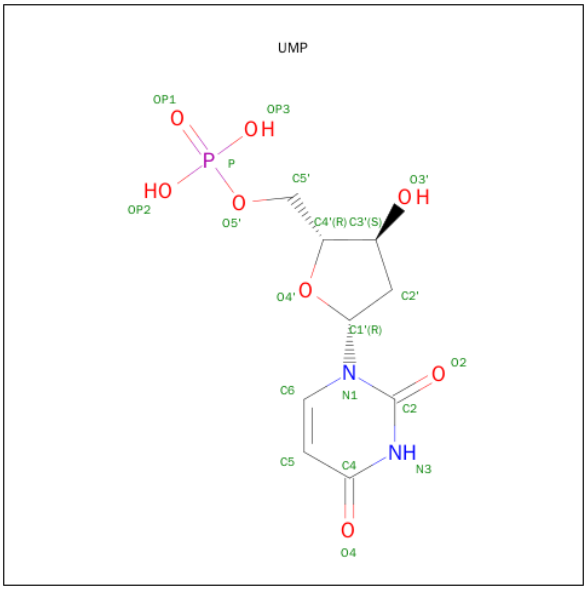
Chain	Residue	Modelled	Actual	Comment	Reference
A	43	CME	CYS	MODIFIED RESIDUE	UNP P04818
B	43	CME	CYS	MODIFIED RESIDUE	UNP P04818
C	43	CME	CYS	MODIFIED RESIDUE	UNP P04818
D	43	CME	CYS	MODIFIED RESIDUE	UNP P04818

- Molecule 2 is TOMUDEX (three-letter code: D16) (formula: $C_{21}H_{22}N_4O_6S$).



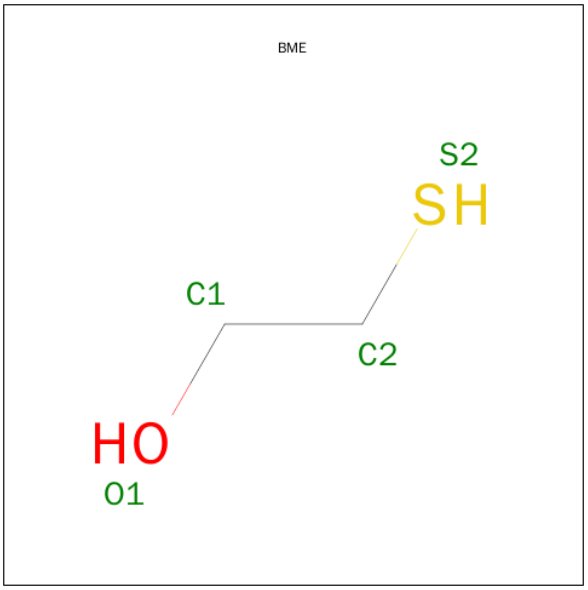
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	C	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	D	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	119	Total	O	0	0
			119	119		

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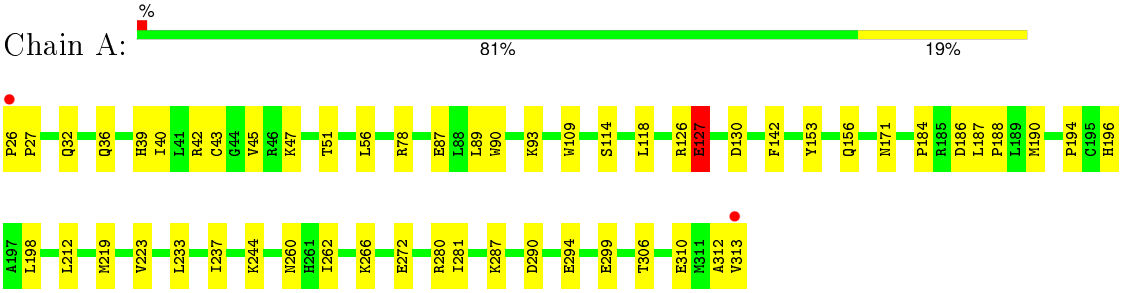
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	151	Total O 151 151	0	0
5	D	170	Total O 170 170	0	0

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.

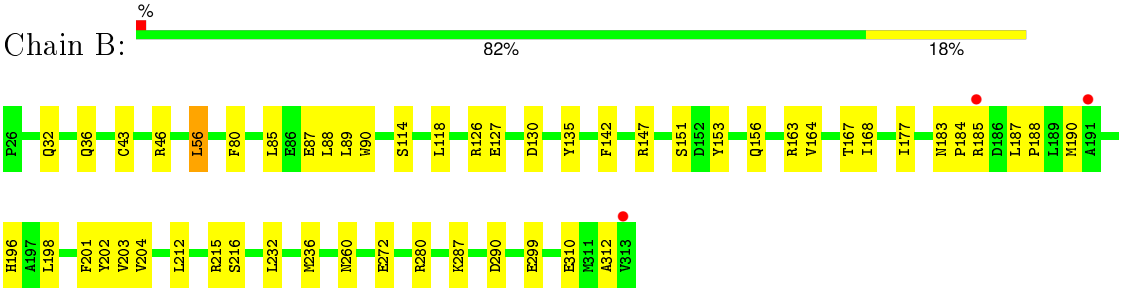
- Molecule 1: THYMIDYLATE SYNTHASE

Chain A:



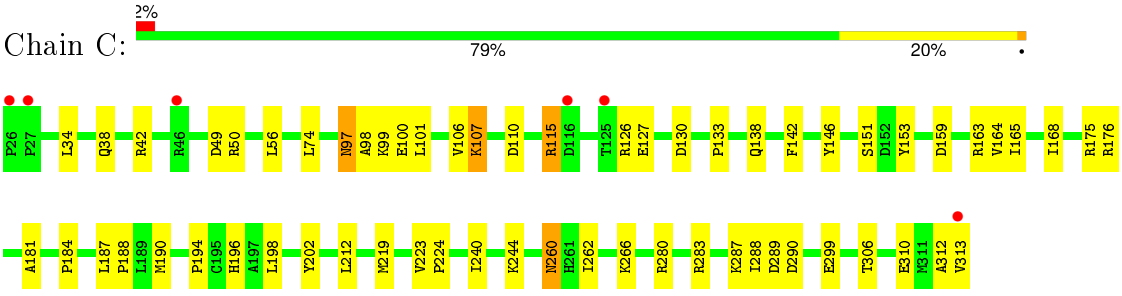
- Molecule 1: THYMIDYLATE SYNTHASE

Chain B:



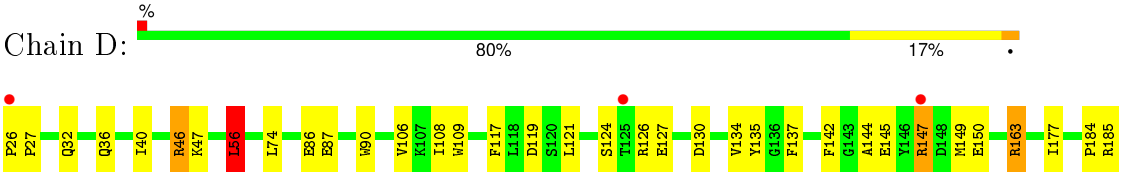
- Molecule 1: THYMIDYLATE SYNTHASE

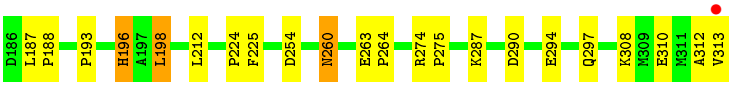
Chain C:



- Molecule 1: THYMIDYLATE SYNTHASE

Chain D:




D186
L187
P188
P193
H196
A197
L198
L212
P224
F225
D254
N260
E263
P264
R274
P275
K287
D290
E294
Q297
K308
M309
E310
M311
A312
V313

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.85Å 70.50Å 74.53Å 70.23° 83.29° 73.28°	Depositor
Resolution (Å)	20.09 – 1.90 70.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	79.2 (20.09-1.90) 83.6 (70.12-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.244 0.209 , 0.246	Depositor DCC
R_{free} test set	6602 reflections (7.03%)	DCC
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 93878 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10136	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: D16, UMP, CME, BME

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	0.37	1/2378 (0.0%)	0.62	1/3213 (0.0%)
1	B	0.36	1/2378 (0.0%)	0.59	1/3213 (0.0%)
1	C	0.37	1/2378 (0.0%)	0.60	1/3213 (0.0%)
1	D	0.37	1/2378 (0.0%)	0.61	1/3213 (0.0%)
All	All	0.36	4/9512 (0.0%)	0.60	4/12852 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	GLU	CD-OE2	7.28	1.33	1.25
1	C	127	GLU	CD-OE2	7.19	1.33	1.25
1	B	127	GLU	CD-OE2	7.10	1.33	1.25
1	A	127	GLU	CD-OE2	7.10	1.33	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	56	LEU	N-CA-C	-5.75	95.49	111.00
1	A	56	LEU	N-CA-C	-5.67	95.70	111.00
1	C	56	LEU	N-CA-C	-5.49	96.18	111.00
1	B	56	LEU	N-CA-C	-5.32	96.63	111.00

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	2329	0	2299	44	0
1	B	2329	0	2299	44	0
1	C	2329	0	2299	46	0
1	D	2329	0	2299	48	0
2	A	32	0	20	1	0
2	B	32	0	20	1	0
2	C	32	0	20	0	0
2	D	32	0	20	1	0
3	A	20	0	10	0	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	4	0	5	0	0
4	B	4	0	5	2	0
4	C	4	0	5	1	0
4	D	4	0	5	1	0
5	A	156	0	0	2	0
5	B	119	0	0	4	0
5	C	151	0	0	3	0
5	D	170	0	0	4	0
All	All	10136	0	9336	170	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 9.

All (170) 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:D:163:ARG:HH11	1:D:163:ARG:HB3	1.18	1.06
1:D:147:ARG:HB3	1:D:147:ARG:HH11	1.26	0.96
1:C:101:LEU:HG	1:C:106:VAL:HG13	1.63	0.81
1:D:163:ARG:NH1	1:D:163:ARG:HB3	1.98	0.79
1:A:78:ARG:HB3	1:A:306:THR:HG22	1.64	0.79
1:C:74:LEU:HD12	1:C:224:PRO:HB3	1.67	0.76
1:D:147:ARG:NH1	1:D:147:ARG:HB3	2.01	0.75
1:D:297:GLN:HG3	5:D:968:HOH:O	1.85	0.74
1:C:107:LYS:HB3	1:C:110:ASP:OD2	1.87	0.74
1:D:260:ASN:HD22	1:D:260:ASN:N	1.87	0.71
1:C:260:ASN:H	1:C:260:ASN:HD22	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASN:HD22	1:C:260:ASN:N	1.89	0.70
1:D:260:ASN:HD22	1:D:260:ASN:H	1.39	0.69
1:D:46:ARG:HD3	1:D:46:ARG:C	2.16	0.66
1:D:193:PRO:HG3	5:D:716:HOH:O	1.96	0.64
1:B:196:HIS:HB3	1:B:212:LEU:HD11	1.80	0.64
1:C:126:ARG:HG2	1:C:130:ASP:HB3	1.80	0.63
1:A:43:CME:HZ2	1:A:43:CME:HA	1.80	0.63
1:B:43:CME:HZ3	1:B:43:CME:HB2	1.79	0.63
1:D:32:GLN:O	1:D:36:GLN:HG3	1.98	0.63
1:C:97:ASN:ND2	1:C:99:LYS:H	1.96	0.63
1:B:153:TYR:HA	1:B:156:GLN:NE2	2.14	0.62
1:B:187:LEU:HA	1:B:190:MET:HE3	1.81	0.62
1:C:159:ASP:O	1:C:163:ARG:HG2	2.00	0.61
1:D:313:VAL:HA	5:D:908:HOH:O	1.99	0.61
1:A:281:ILE:N	1:A:281:ILE:HD12	2.15	0.61
1:A:312:ALA:O	1:A:313:VAL:HB	2.01	0.60
1:A:51:THR:HB	1:A:313:VAL:HA	1.83	0.60
1:C:163:ARG:HB3	4:C:1516:BME:H21	1.83	0.60
1:C:115:ARG:HG3	1:C:115:ARG:HH11	1.67	0.60
1:A:190:MET:SD	1:A:194:PRO:HD3	2.43	0.59
1:A:294:GLU:H	1:A:294:GLU:CD	2.06	0.59
1:B:198:LEU:HD12	1:B:198:LEU:C	2.22	0.58
1:C:262:ILE:O	1:C:266:LYS:HG3	2.04	0.58
1:D:260:ASN:ND2	1:D:260:ASN:H	2.02	0.57
1:B:147:ARG:NH1	1:B:151:SER:HB3	2.20	0.57
1:A:89:LEU:O	1:A:93:LYS:HG3	2.04	0.57
1:C:288:ILE:HG23	1:C:289:ASP:OD2	2.05	0.56
1:D:198:LEU:HD12	1:D:198:LEU:C	2.26	0.56
1:C:133:PRO:HG3	1:C:146:TYR:CG	2.40	0.56
1:C:190:MET:SD	1:C:194:PRO:HD3	2.46	0.56
1:D:74:LEU:HD22	1:D:224:PRO:HB3	1.87	0.56
1:A:45:VAL:CG2	1:B:204:VAL:HG21	2.35	0.56
1:A:233:LEU:O	1:A:237:ILE:HD13	2.05	0.56
1:B:32:GLN:O	1:B:36:GLN:HG3	2.07	0.55
1:B:290:ASP:HB3	5:B:659:HOH:O	2.06	0.55
1:A:32:GLN:O	1:A:36:GLN:HG3	2.06	0.54
1:C:260:ASN:H	1:C:260:ASN:ND2	2.04	0.54
1:A:42:ARG:NH1	1:A:43:CME:SG	2.81	0.54
1:A:313:VAL:HG13	1:A:313:VAL:O	2.08	0.54
1:A:45:VAL:HG21	1:B:204:VAL:HG21	1.89	0.54
1:C:196:HIS:HB3	1:C:212:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LEU:N	1:D:188:PRO:HD2	2.23	0.54
1:B:147:ARG:HB2	1:B:151:SER:OG	2.07	0.54
1:A:90:TRP:HA	1:A:93:LYS:HD3	1.91	0.53
1:A:127:GLU:HG2	5:A:673:HOH:O	2.07	0.53
1:D:312:ALA:HB2	5:D:621:HOH:O	2.09	0.53
1:C:34:LEU:O	1:C:38:GLN:HG3	2.09	0.53
1:D:260:ASN:ND2	1:D:260:ASN:N	2.57	0.53
1:D:196:HIS:CB	1:D:212:LEU:HD11	2.38	0.53
1:A:187:LEU:N	1:A:188:PRO:HD2	2.24	0.53
1:C:142:PHE:CE2	1:D:184:PRO:HD2	2.44	0.52
1:C:165:ILE:HD13	1:C:240:ILE:HD11	1.90	0.52
1:C:187:LEU:N	1:C:188:PRO:HD2	2.24	0.52
1:C:223:VAL:HB	1:C:224:PRO:HD3	1.92	0.51
1:A:196:HIS:HB3	1:A:212:LEU:HD11	1.93	0.51
1:C:42:ARG:HD3	5:C:704:HOH:O	2.11	0.51
1:D:87:GLU:OE1	1:D:225:PHE:HE2	1.94	0.51
1:A:198:LEU:HD12	1:A:198:LEU:C	2.31	0.51
1:B:126:ARG:HD3	1:B:130:ASP:O	2.11	0.50
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.45	0.50
1:D:119:ASP:OD1	1:D:124:SER:HA	2.11	0.50
1:D:308:LYS:HE3	1:D:310:GLU:OE2	2.11	0.50
1:A:36:GLN:O	1:A:40:ILE:HG13	2.12	0.50
1:C:260:ASN:ND2	1:C:260:ASN:N	2.59	0.50
1:C:38:GLN:O	1:C:42:ARG:HG2	2.12	0.50
1:B:312:ALA:HB3	2:B:415:D16:HM22	1.93	0.50
1:B:215:ARG:HG3	1:B:216:SER:N	2.27	0.50
1:A:313:VAL:O	1:A:313:VAL:HG22	2.11	0.50
1:B:114:SER:O	1:B:118:LEU:HG	2.12	0.50
1:C:198:LEU:HD12	1:C:198:LEU:C	2.33	0.50
1:B:312:ALA:HB2	5:B:669:HOH:O	2.11	0.49
1:A:153:TYR:HA	1:A:156:GLN:OE1	2.13	0.49
1:C:175:ARG:HG2	1:D:254:ASP:OD2	2.12	0.49
1:D:163:ARG:CB	1:D:163:ARG:HH11	2.06	0.49
1:B:147:ARG:HH11	1:B:151:SER:HB3	1.78	0.48
1:B:43:CME:HZ3	1:B:43:CME:CB	2.44	0.48
1:C:97:ASN:C	1:C:97:ASN:HD22	2.17	0.48
1:B:183:ASN:HD21	1:B:185:ARG:NH1	2.12	0.47
1:A:109:TRP:CZ2	2:A:414:D16:H91	2.49	0.47
1:B:183:ASN:OD1	1:B:185:ARG:HG3	2.14	0.47
1:D:263:GLU:HB2	1:D:264:PRO:HD3	1.96	0.47
1:C:312:ALA:HA	5:C:646:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:MET:SD	1:C:223:VAL:HG21	2.55	0.47
1:C:202:TYR:CE1	1:D:47:LYS:HE2	2.50	0.47
1:D:87:GLU:O	1:D:90:TRP:HB3	2.14	0.47
1:B:280:ARG:HE	1:B:299:GLU:CD	2.18	0.47
1:D:294:GLU:CD	1:D:294:GLU:H	2.16	0.47
1:C:287:LYS:HB2	1:C:290:ASP:OD1	2.15	0.47
1:A:184:PRO:HD2	1:B:142:PHE:CE2	2.50	0.47
1:A:280:ARG:HE	1:A:299:GLU:CD	2.18	0.46
1:B:85:LEU:O	1:B:89:LEU:HG	2.15	0.46
1:D:106:VAL:HG12	1:D:108:ILE:HG12	1.97	0.46
1:A:47:LYS:HE3	1:B:202:TYR:CE1	2.49	0.46
1:C:176:ARG:HD3	1:D:193:PRO:HG2	1.98	0.46
1:B:151:SER:HB2	1:B:153:TYR:CZ	2.51	0.46
1:A:312:ALA:O	1:A:313:VAL:CB	2.64	0.46
1:A:262:ILE:O	1:A:266:LYS:HG3	2.16	0.45
1:D:126:ARG:HD3	1:D:130:ASP:O	2.15	0.45
1:D:149:MET:HG3	1:D:150:GLU:HG3	1.98	0.45
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.81	0.45
1:C:151:SER:HB2	1:C:153:TYR:CZ	2.51	0.45
1:A:287:LYS:O	1:A:290:ASP:HB2	2.17	0.45
1:B:287:LYS:HE2	5:B:711:HOH:O	2.17	0.45
1:C:142:PHE:CZ	1:D:184:PRO:HD2	2.52	0.45
1:B:88:LEU:HD23	1:B:232:LEU:HG	1.98	0.45
1:A:39:HIS:O	1:A:43:CME:N	2.49	0.45
1:C:107:LYS:N	1:C:107:LYS:HD2	2.32	0.45
1:D:117:PHE:CE1	1:D:121:LEU:HD11	2.52	0.45
1:D:46:ARG:HD3	1:D:47:LYS:N	2.33	0.44
1:C:280:ARG:HE	1:C:299:GLU:CD	2.20	0.44
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.98	0.44
1:B:187:LEU:N	1:B:188:PRO:CD	2.80	0.44
1:B:87:GLU:O	1:B:90:TRP:HB3	2.18	0.44
1:A:237:ILE:N	1:A:237:ILE:HD12	2.33	0.44
1:B:287:LYS:HB2	1:B:290:ASP:OD1	2.18	0.43
1:C:97:ASN:HD22	1:C:98:ALA:N	2.17	0.43
1:C:184:PRO:HD2	1:D:142:PHE:CE2	2.52	0.43
1:B:88:LEU:HD23	1:B:236:MET:HE1	1.99	0.43
1:D:86:GLU:HB2	1:D:106:VAL:HG21	2.00	0.43
1:B:232:LEU:HG	1:B:236:MET:HE3	2.01	0.43
1:B:177:ILE:CG2	1:B:201:PHE:HB2	2.48	0.43
1:D:145:GLU:OE1	1:D:185:ARG:NH2	2.51	0.43
1:A:260:ASN:ND2	1:A:310:GLU:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:N	1:A:27:PRO:HD3	2.34	0.43
1:C:164:VAL:O	1:C:168:ILE:HG13	2.19	0.43
1:A:87:GLU:O	1:A:90:TRP:HB3	2.19	0.43
1:C:50:ARG:HG2	1:C:50:ARG:HH11	1.84	0.43
1:C:313:VAL:HG22	1:C:313:VAL:OXT	2.19	0.43
1:D:26:PRO:HA	1:D:27:PRO:HD3	1.96	0.42
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.84	0.42
1:C:283:ARG:HD2	5:C:713:HOH:O	2.18	0.42
1:B:167:THR:HG21	4:B:1515:BME:H11	2.00	0.42
1:A:45:VAL:HG23	1:B:204:VAL:HG21	2.02	0.42
1:B:164:VAL:O	1:B:168:ILE:HG13	2.20	0.42
1:D:177:ILE:HA	4:D:1517:BME:H12	2.02	0.42
1:B:287:LYS:HB3	5:B:711:HOH:O	2.20	0.41
1:D:109:TRP:CZ2	2:D:417:D16:H91	2.55	0.41
1:C:138:GLN:HG3	1:C:181:ALA:O	2.20	0.41
1:A:186:ASP:C	1:A:188:PRO:HD2	2.41	0.41
1:B:183:ASN:HD21	1:B:185:ARG:HH12	1.68	0.41
1:B:164:VAL:HG13	1:B:177:ILE:CG2	2.51	0.41
1:D:287:LYS:HB2	1:D:290:ASP:OD1	2.20	0.41
1:D:145:GLU:HA	1:D:145:GLU:OE1	2.20	0.41
1:D:274:ARG:O	1:D:275:PRO:C	2.58	0.41
1:C:126:ARG:CG	1:C:130:ASP:HB3	2.48	0.41
1:D:196:HIS:HB2	1:D:212:LEU:HD11	2.02	0.41
1:B:163:ARG:HG3	4:B:1515:BME:H22	2.02	0.41
1:A:171:ASN:ND2	5:A:688:HOH:O	2.52	0.41
1:C:244:LYS:HE2	1:C:244:LYS:HB2	1.94	0.41
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.85	0.41
1:B:168:ILE:HG23	1:B:203:VAL:HG21	2.02	0.41
1:A:219:MET:SD	1:A:223:VAL:HG21	2.61	0.41
1:D:137:PHE:CZ	1:D:144:ALA:HB3	2.56	0.41
1:D:36:GLN:O	1:D:40:ILE:HG13	2.21	0.41
1:B:187:LEU:HD23	1:B:190:MET:CE	2.51	0.41
1:A:114:SER:O	1:A:118:LEU:HG	2.20	0.41
1:A:281:ILE:CD1	1:A:281:ILE:N	2.82	0.40
1:A:126:ARG:CG	1:A:130:ASP:HB3	2.52	0.40
1:C:97:ASN:HB3	1:C:100:GLU:HG3	2.03	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	285/288 (99%)	271 (95%)	14 (5%)	0	100	100
1	B	285/288 (99%)	272 (95%)	11 (4%)	2 (1%)	26	14
1	C	285/288 (99%)	272 (95%)	13 (5%)	0	100	100
1	D	285/288 (99%)	266 (93%)	17 (6%)	2 (1%)	26	14
All	All	1140/1152 (99%)	1081 (95%)	55 (5%)	4 (0%)	39	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	TYR
1	D	135	TYR
1	B	80	PHE
1	D	134	VAL

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	250/250 (100%)	248 (99%)	2 (1%)	86	86
1	B	250/250 (100%)	245 (98%)	5 (2%)	63	57
1	C	250/250 (100%)	243 (97%)	7 (3%)	51	41
1	D	250/250 (100%)	243 (97%)	7 (3%)	51	41
All	All	1000/1000 (100%)	979 (98%)	21 (2%)	61	55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLU
1	A	272	GLU
1	B	46	ARG
1	B	56	LEU
1	B	260	ASN
1	B	272	GLU
1	B	310	GLU
1	C	49	ASP
1	C	97	ASN
1	C	107	LYS
1	C	115	ARG
1	C	260	ASN
1	C	306	THR
1	C	310	GLU
1	D	46	ARG
1	D	56	LEU
1	D	147	ARG
1	D	163	ARG
1	D	196	HIS
1	D	198	LEU
1	D	260	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	171	ASN
1	A	196	HIS
1	A	200	GLN
1	A	211	GLN
1	B	112	ASN
1	B	156	GLN
1	B	196	HIS
1	B	200	GLN
1	B	211	GLN
1	B	260	ASN
1	B	302	ASN
1	C	97	ASN
1	C	171	ASN
1	C	196	HIS
1	C	200	GLN

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Mol	Chain	Res	Type
1	C	260	ASN
1	C	297	GLN
1	C	302	ASN
1	D	38	GLN
1	D	171	ASN
1	D	200	GLN
1	D	211	GLN
1	D	260	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
1	CME	A	43	1	8,9,10	0.49	0	6,9,11	0.95	1 (16%)
1	CME	B	43	1	8,9,10	0.42	0	6,9,11	0.97	1 (16%)
1	CME	C	43	1	8,9,10	0.44	0	6,9,11	0.90	0
1	CME	D	43	1	8,9,10	0.41	0	6,9,11	0.98	1 (16%)

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
1	CME	A	43	1	-	0/5/8/10	0/0/0/0
1	CME	B	43	1	-	0/5/8/10	0/0/0/0
1	CME	C	43	1	-	0/5/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	D	43	1	-	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})
1	B	43	CME	O-C-CA	-2.20	119.76	125.49
1	A	43	CME	O-C-CA	-2.17	119.84	125.49
1	D	43	CME	O-C-CA	-2.15	119.88	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	43	CME	3	0
1	B	43	CME	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 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	BME	A	1514	-	3,3,3	1.92	1 (33%)	2,2,2	1.75	1 (50%)
3	UMP	A	314	1	16,21,21	3.41	6 (37%)	23,31,31	2.75	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	D16	A	414	-	25,34,34	1.73	4 (16%)	22,48,48	2.01	5 (22%)
4	BME	B	1515	-	3,3,3	1.90	1 (33%)	2,2,2	1.74	1 (50%)
3	UMP	B	315	1	16,21,21	3.35	7 (43%)	23,31,31	2.73	4 (17%)
2	D16	B	415	-	25,34,34	1.78	5 (20%)	22,48,48	2.04	6 (27%)
4	BME	C	1516	-	3,3,3	1.94	1 (33%)	2,2,2	1.68	1 (50%)
3	UMP	C	316	1	16,21,21	3.30	6 (37%)	23,31,31	2.76	3 (13%)
2	D16	C	416	-	25,34,34	1.67	4 (16%)	22,48,48	2.14	6 (27%)
4	BME	D	1517	-	3,3,3	1.91	1 (33%)	2,2,2	1.74	1 (50%)
3	UMP	D	317	1	16,21,21	3.35	7 (43%)	23,31,31	2.78	5 (21%)
2	D16	D	417	-	25,34,34	1.76	5 (20%)	22,48,48	2.04	6 (27%)

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	BME	A	1514	-	-	0/1/1/1	0/0/0/0
3	UMP	A	314	1	-	0/6/22/22	0/2/2/2
2	D16	A	414	-	-	0/13/25/25	0/3/3/3
4	BME	B	1515	-	-	0/1/1/1	0/0/0/0
3	UMP	B	315	1	-	0/6/22/22	0/2/2/2
2	D16	B	415	-	-	0/13/25/25	0/3/3/3
4	BME	C	1516	-	-	0/1/1/1	0/0/0/0
3	UMP	C	316	1	-	0/6/22/22	0/2/2/2
2	D16	C	416	-	-	0/13/25/25	0/3/3/3
4	BME	D	1517	-	-	0/1/1/1	0/0/0/0
3	UMP	D	317	1	-	0/6/22/22	0/2/2/2
2	D16	D	417	-	-	0/13/25/25	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	316	UMP	C3'-C4'	-4.29	1.40	1.53
3	D	317	UMP	C3'-C4'	-4.23	1.41	1.53
3	B	315	UMP	C3'-C4'	-4.07	1.41	1.53
3	A	314	UMP	C3'-C4'	-4.02	1.41	1.53
4	C	1516	BME	O1-C1	-3.34	1.24	1.42
4	A	1514	BME	O1-C1	-3.29	1.24	1.42
4	D	1517	BME	O1-C1	-3.28	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1515	BME	O1-C1	-3.24	1.24	1.42
3	A	314	UMP	P-OP3	-2.45	1.45	1.54
3	D	317	UMP	P-OP3	-2.45	1.45	1.54
3	D	317	UMP	O4'-C1'	-2.40	1.36	1.42
3	C	316	UMP	P-OP3	-2.38	1.46	1.54
3	A	314	UMP	P-OP2	-2.32	1.46	1.54
3	C	316	UMP	P-OP2	-2.32	1.46	1.54
3	B	315	UMP	P-OP3	-2.30	1.46	1.54
3	B	315	UMP	O4'-C1'	-2.24	1.37	1.42
3	D	317	UMP	P-OP2	-2.21	1.46	1.54
3	B	315	UMP	P-OP2	-2.02	1.47	1.54
2	D	417	D16	C7-C6	2.15	1.43	1.38
2	B	415	D16	C7-C6	2.28	1.43	1.38
2	B	415	D16	C16-C15	2.29	1.50	1.39
2	C	416	D16	C16-C15	2.30	1.50	1.39
2	A	414	D16	C16-C15	2.37	1.51	1.39
2	D	417	D16	C16-C15	2.39	1.51	1.39
3	C	316	UMP	C6-C5	2.58	1.43	1.38
3	A	314	UMP	C6-C5	2.63	1.43	1.38
2	C	416	D16	C8-C7	2.82	1.42	1.36
2	B	415	D16	C5-C6	2.84	1.44	1.37
3	B	315	UMP	C6-C5	2.87	1.44	1.38
2	B	415	D16	C8-C7	2.88	1.42	1.36
3	D	317	UMP	C6-C5	2.97	1.44	1.38
2	D	417	D16	C5-C6	2.98	1.44	1.37
2	A	414	D16	C8-C7	3.00	1.42	1.36
2	A	414	D16	C5-C6	3.05	1.44	1.37
2	D	417	D16	C8-C7	3.17	1.43	1.36
2	C	416	D16	C5-C6	3.39	1.45	1.37
3	A	314	UMP	C4-N3	3.61	1.39	1.33
3	C	316	UMP	C4-N3	3.61	1.39	1.33
3	D	317	UMP	C4-N3	3.77	1.40	1.33
3	B	315	UMP	C4-N3	3.79	1.40	1.33
2	C	416	D16	O4-C4	4.92	1.36	1.24
2	A	414	D16	O4-C4	5.28	1.37	1.24
2	D	417	D16	O4-C4	5.30	1.37	1.24
2	B	415	D16	O4-C4	5.58	1.38	1.24
3	C	316	UMP	C6-N1	10.88	1.51	1.35
3	D	317	UMP	C6-N1	10.91	1.51	1.35
3	B	315	UMP	C6-N1	11.11	1.51	1.35
3	A	314	UMP	C6-N1	11.47	1.51	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	314	UMP	C5-C6-N1	-3.56	111.86	120.58
3	C	316	UMP	C5-C6-N1	-3.55	111.89	120.58
3	B	315	UMP	C5-C6-N1	-3.36	112.35	120.58
3	D	317	UMP	C5-C6-N1	-3.27	112.56	120.58
2	C	416	D16	N1-C2-N3	-2.79	120.10	125.58
2	B	415	D16	N1-C2-N3	-2.78	120.10	125.58
2	D	417	D16	N1-C2-N3	-2.76	120.15	125.58
2	A	414	D16	N1-C2-N3	-2.74	120.19	125.58
2	C	416	D16	C4-C4A-C8A	-2.56	116.05	118.54
3	D	317	UMP	O4'-C1'-C2'	-2.38	101.53	106.27
3	B	315	UMP	O4'-C1'-C2'	-2.24	101.82	106.27
2	B	415	D16	C4-C4A-C8A	-2.10	116.50	118.54
2	D	417	D16	C4-C4A-C8A	-2.07	116.53	118.54
3	D	317	UMP	C4'-O4'-C1'	2.04	114.63	109.47
2	A	414	D16	CM2-C2-N1	2.21	120.97	117.21
4	C	1516	BME	O1-C1-C2	2.33	121.03	110.83
2	B	415	D16	CM2-C2-N1	2.34	121.19	117.21
4	D	1517	BME	O1-C1-C2	2.40	121.35	110.83
4	B	1515	BME	O1-C1-C2	2.41	121.37	110.83
2	C	416	D16	CM2-C2-N1	2.42	121.31	117.21
4	A	1514	BME	O1-C1-C2	2.44	121.51	110.83
2	D	417	D16	CM2-C2-N1	2.49	121.44	117.21
2	D	417	D16	C6-C9-N10	3.02	116.86	113.03
2	A	414	D16	C6-C9-N10	3.31	117.22	113.03
2	C	416	D16	C6-C9-N10	3.68	117.70	113.03
2	B	415	D16	C6-C9-N10	4.01	118.11	113.03
3	D	317	UMP	O4'-C1'-N1	4.05	114.72	107.72
3	B	315	UMP	O4'-C1'-N1	4.10	114.82	107.72
2	B	415	D16	CG-CB-CA	4.48	122.08	112.99
2	B	415	D16	C2-N1-C8A	4.50	120.94	115.86
2	A	414	D16	CG-CB-CA	4.57	122.27	112.99
2	D	417	D16	C2-N1-C8A	4.69	121.14	115.86
3	C	316	UMP	O4'-C1'-N1	4.71	115.86	107.72
2	C	416	D16	CG-CB-CA	4.73	122.60	112.99
2	A	414	D16	C2-N1-C8A	4.78	121.25	115.86
3	A	314	UMP	O4'-C1'-N1	4.80	116.02	107.72
2	C	416	D16	C2-N1-C8A	5.06	121.57	115.86
2	D	417	D16	CG-CB-CA	5.20	123.55	112.99
3	A	314	UMP	C4-N3-C2	10.80	124.84	114.14
3	C	316	UMP	C4-N3-C2	10.85	124.89	114.14
3	B	315	UMP	C4-N3-C2	10.89	124.93	114.14
3	D	317	UMP	C4-N3-C2	11.11	125.14	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	414	D16	1	0
4	B	1515	BME	2	0
2	B	415	D16	1	0
4	C	1516	BME	1	0
4	D	1517	BME	1	0
2	D	417	D16	1	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	287/288 (99%)	-0.06	2 (0%)	89	90	9, 19, 35, 41	0
1	B	287/288 (99%)	-0.02	3 (1%)	84	86	10, 23, 38, 50	0
1	C	287/288 (99%)	-0.08	6 (2%)	67	70	8, 19, 36, 49	0
1	D	287/288 (99%)	-0.08	4 (1%)	78	80	9, 20, 35, 50	0
All	All	1148/1152 (99%)	-0.06	15 (1%)	79	82	8, 20, 36, 50	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	VAL	8.6
1	A	313	VAL	6.7
1	C	26	PRO	6.0
1	D	313	VAL	4.8
1	C	313	VAL	3.5
1	A	26	PRO	3.3
1	B	185	ARG	3.2
1	B	191	ALA	3.0
1	C	27	PRO	2.9
1	D	125	THR	2.6
1	D	26	PRO	2.5
1	D	147	ARG	2.5
1	C	46	ARG	2.5
1	C	116	ASP	2.5
1	C	125	THR	2.3

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

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
1	CME	B	43	10/11	0.97	0.10	-	21,24,36,38	0
1	CME	C	43	10/11	0.91	0.14	-	28,32,44,45	0
1	CME	A	43	10/11	0.92	0.15	-	28,29,42,44	0
1	CME	D	43	10/11	0.97	0.09	-	19,21,26,27	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
4	BME	A	1514	4/4	0.77	0.18	5.13	34,36,36,37	0
4	BME	C	1516	4/4	0.79	0.23	4.53	50,52,52,53	0
4	BME	D	1517	4/4	0.57	0.20	2.77	47,48,49,50	0
2	D16	C	416	32/32	0.92	0.15	1.53	12,26,47,49	0
4	BME	B	1515	4/4	0.74	0.17	1.47	40,41,42,42	0
2	D16	A	414	32/32	0.91	0.13	0.79	14,22,39,41	0
2	D16	B	415	32/32	0.89	0.14	0.66	16,26,43,44	0
3	UMP	A	314	20/20	0.96	0.10	0.39	13,15,18,21	0
3	UMP	B	315	20/20	0.95	0.10	0.16	11,16,19,21	0
2	D16	D	417	32/32	0.92	0.12	0.14	15,19,35,36	0
3	UMP	D	317	20/20	0.98	0.09	-0.33	8,14,16,21	0
3	UMP	C	316	20/20	0.96	0.09	-0.43	8,13,16,21	0

6.5 Other polymers (i)

There are no such residues in this entry.