Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 09:15 AM EDT

PDB ID	:	2WYA
Title	:	CRYSTAL STRUCTURE OF HUMAN MITOCHONDRIAL 3-HYDROXY-3 -METHYLGLUTARYL- COENZYME A SYNTHASE 2 (HMGCS2)
Authors	:	Yue, W.W.; Shafqat, N.; Savitsky, P.; Roos, A.K.; Cooper, C.; Murray, J.W.; von Delft, F.; Arrowsmith, C.; Wikstrom, M.; Edwards, A.; Bountra, C.; Oppermann, U.
Deposited on	:	2009-11-13
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

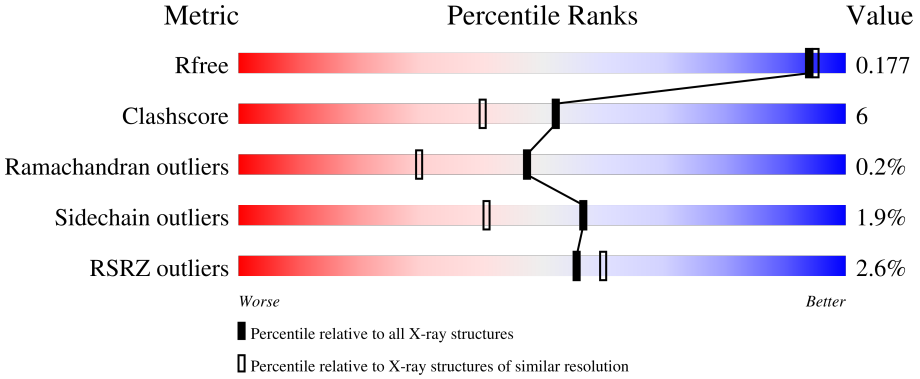
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	2% 89% 10% •
1	B	460	2% 88% 11% •
1	C	460	2% 91% 8% •
1	D	460	3% 89% 10% •

2 Entry composition (i)

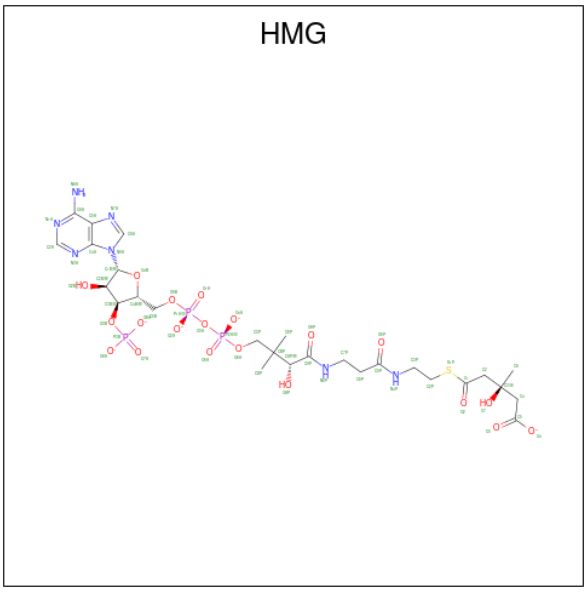
There are 4 unique types of molecules in this entry. The entry contains 16074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYDROXYMETHYLGLUTARYL-COA SYNTHASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	3589	2265	609	691	24	0	8	0
1	B	460	3606	2277	610	694	25	0	9	0
1	C	460	3569	2254	600	690	25	0	7	0
1	D	460	3615	2283	611	695	26	0	13	0

- Molecule 2 is 3-HYDROXY-3-METHYLGLUTARYL-COENZYME A (three-letter code: HMG) (formula: $C_{27}H_{39}N_7O_{20}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	58	27	7	20	3	1	0	0

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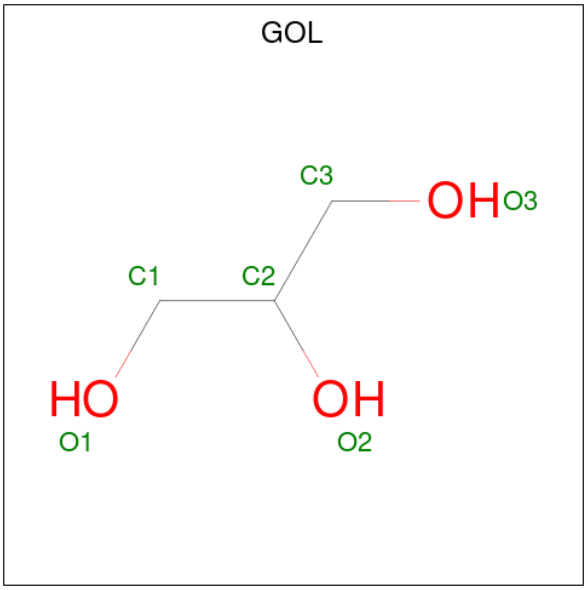
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	B	1	58	27	7	20	3	1	0	0
			Total	C	N	O	P	S		
2	C	1	58	27	7	20	3	1	0	0
			Total	C	N	O	P	S		
2	D	1	58	27	7	20	3	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0

- Molecule 4 is water.

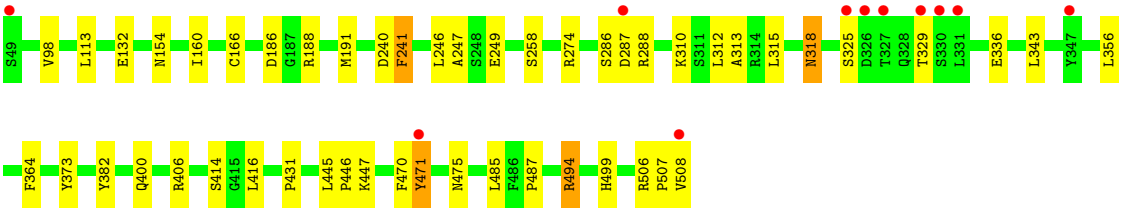
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	365	365	365	0	0
			Total	O		
4	B	384	384	384	0	0
			Total	O		
4	C	358	358	358	0	0
			Total	O		
4	D	350	350	350	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

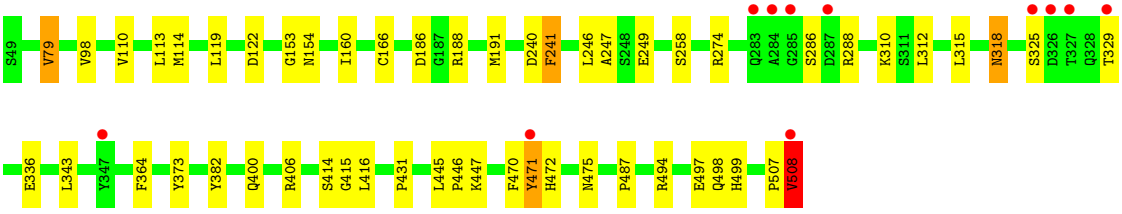
• Molecule 1: HYDROXYMETHYLGLUTARYL-COA SYNTHASE, MITOCHONDRIAL

Chain A:



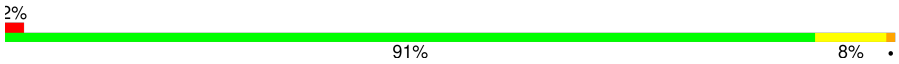
• Molecule 1: HYDROXYMETHYLGLUTARYL-COA SYNTHASE, MITOCHONDRIAL

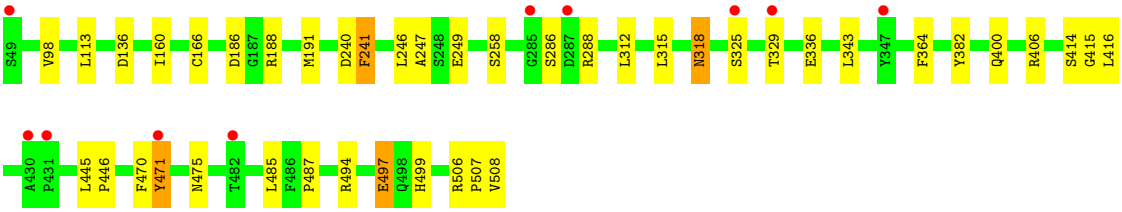
Chain B:



• Molecule 1: HYDROXYMETHYLGLUTARYL-COA SYNTHASE, MITOCHONDRIAL

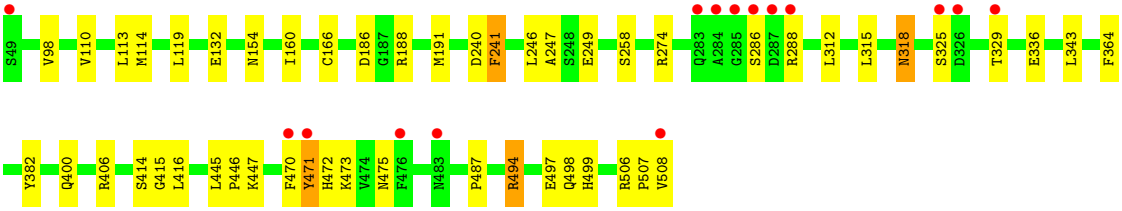
Chain C:





• Molecule 1: HYDROXYMETHYLGLUTARYL-COA SYNTHASE, MITOCHONDRIAL

Chain D:


S49
V98
V110
L113
M114
L119
E132
N154
I160
C166
D186
G187
R188
M191
D240
F241
L246
A247
S248
E249
S258
R274
Q283
A284
G285
S286
D287
R288
L312
L315
N318
S325
D326
T329
E336
L343
F364
Y382
Q400
R406
S414
G415
L416
L445
P446
K447
F470
Y471
H472
K473
V474
N475
F476
M483
P487
R494
E497
Q498
H499
R506
P507
V508

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.41Å 83.51Å 101.44Å 100.00° 108.08° 96.30°	Depositor
Resolution (Å)	31.36 – 1.70 31.36 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (31.36-1.70) 88.3 (31.36-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.161 , 0.184 0.155 , 0.177	Depositor DCC
R_{free} test set	1764 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16074	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2596e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, HMG

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	0.39	2/3689 (0.1%)	0.57	3/4996 (0.1%)
1	B	0.40	2/3711 (0.1%)	0.60	5/5025 (0.1%)
1	C	0.43	5/3666 (0.1%)	0.63	6/4967 (0.1%)
1	D	0.39	2/3731 (0.1%)	0.57	3/5053 (0.1%)
All	All	0.41	11/14797 (0.1%)	0.59	17/20041 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	406	ARG	CZ-NH1	-7.89	1.22	1.33
1	B	406	ARG	CZ-NH1	-7.70	1.23	1.33
1	C	406	ARG	CZ-NH2	-7.35	1.23	1.33
1	C	497	GLU	CD-OE2	7.01	1.33	1.25
1	A	406	ARG	CZ-NH2	-6.94	1.24	1.33
1	C	406	ARG	CZ-NH1	-6.93	1.24	1.33
1	B	406	ARG	CZ-NH2	-6.90	1.24	1.33
1	A	406	ARG	CZ-NH1	-6.79	1.24	1.33
1	D	406	ARG	CZ-NH2	-6.57	1.24	1.33
1	C	136	ASP	CG-OD2	-5.97	1.11	1.25
1	C	136	ASP	CG-OD1	-5.83	1.11	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	406	ARG	NE-CZ-NH2	12.78	126.69	120.30
1	D	406	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	C	136	ASP	CB-CG-OD2	11.00	128.20	118.30
1	C	136	ASP	CB-CG-OD1	10.87	128.09	118.30
1	C	406	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	C	136	ASP	OD1-CG-OD2	-10.31	103.70	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	406	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	406	ARG	NE-CZ-NH2	8.98	124.79	120.30
1	C	406	ARG	NH1-CZ-NH2	-8.65	109.88	119.40
1	C	406	ARG	NE-CZ-NH2	8.55	124.57	120.30
1	A	406	ARG	NH1-CZ-NH2	-8.46	110.09	119.40
1	B	406	ARG	NH1-CZ-NH2	-8.35	110.21	119.40
1	D	406	ARG	NH1-CZ-NH2	-8.24	110.34	119.40
1	B	79	VAL	CG1-CB-CG2	7.22	122.45	110.90
1	D	406	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	406	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	508	VAL	CG1-CB-CG2	5.48	119.67	110.90

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	3589	0	3479	44	0
1	B	3606	0	3497	53	0
1	C	3569	0	3449	31	0
1	D	3615	0	3513	42	0
2	A	58	0	39	3	0
2	B	58	0	39	3	0
2	C	58	0	39	1	0
2	D	58	0	39	2	0
3	A	6	0	8	0	0
4	A	365	0	0	5	0
4	B	384	0	0	2	0
4	C	358	0	0	2	0
4	D	350	0	0	4	0
All	All	16074	0	14102	158	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 6.

All (158) 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:B:114[B]:MET:SD	1:B:119:LEU:HD23	1.99	1.02
1:A:400:GLN:HG2	1:B:431:PRO:HG3	1.43	0.97
1:D:114[B]:MET:SD	1:D:119:LEU:HD23	2.04	0.97
1:A:431:PRO:HG3	1:B:400:GLN:HG2	1.45	0.97
1:B:475:ASN:HD22	1:B:497:GLU:HG3	1.32	0.94
1:B:475:ASN:ND2	1:B:497:GLU:HG3	1.83	0.93
1:C:249:GLU:HG3	1:C:471:TYR:CE2	2.21	0.75
1:D:249:GLU:HG3	1:D:471:TYR:CE2	2.22	0.73
1:A:431:PRO:CG	1:B:400:GLN:HG2	2.19	0.71
1:A:400:GLN:HG2	1:B:431:PRO:CG	2.19	0.71
1:B:487:PRO:HB3	1:B:508:VAL:HG22	1.74	0.70
1:B:497:GLU:CD	1:B:497:GLU:H	1.95	0.69
1:A:507:PRO:O	1:A:508:VAL:HB	1.93	0.68
1:C:318[A]:ASN:CG	4:C:2228:HOH:O	2.31	0.68
1:D:507:PRO:O	1:D:508:VAL:HB	1.94	0.67
1:C:507:PRO:O	1:C:508:VAL:HB	1.93	0.66
1:D:497:GLU:HG2	1:D:498:GLN:OE1	1.95	0.66
1:A:249:GLU:HG3	1:A:471:TYR:CE2	2.31	0.65
1:B:498:GLN:HG3	4:B:2367:HOH:O	1.96	0.65
1:A:286:SER:OG	1:A:288[A]:ARG:HG2	1.98	0.63
1:D:497:GLU:H	1:D:497:GLU:CD	2.01	0.63
1:D:286:SER:OG	1:D:288[A]:ARG:HG2	1.97	0.63
1:B:487:PRO:CB	1:B:508:VAL:HG22	2.27	0.63
1:B:318[A]:ASN:HD22	1:B:343:LEU:HD21	1.62	0.63
1:C:318[A]:ASN:HD22	1:C:343:LEU:HD21	1.62	0.63
1:D:498:GLN:HG3	4:D:2336:HOH:O	1.98	0.63
1:A:508:VAL:HG12	4:A:2359:HOH:O	1.98	0.63
1:A:318[A]:ASN:HD22	1:A:343:LEU:HD21	1.64	0.62
1:B:249:GLU:HG3	1:B:471:TYR:CE2	2.36	0.61
1:A:329:THR:HG22	1:A:336:GLU:OE2	2.01	0.60
1:C:249:GLU:HG3	1:C:471:TYR:HE2	1.64	0.60
1:A:247:ALA:HB2	1:D:247:ALA:HB2	1.83	0.60
1:C:497:GLU:H	1:C:497:GLU:CD	2.05	0.60
1:B:247:ALA:HB2	1:C:247:ALA:HB2	1.83	0.60
1:D:329:THR:HG22	1:D:336:GLU:OE2	2.02	0.60
1:D:508:VAL:HG12	4:D:2147:HOH:O	2.01	0.59
1:C:329:THR:HG22	1:C:336:GLU:OE2	2.02	0.59
1:D:318[A]:ASN:HD22	1:D:343:LEU:HD21	1.68	0.59
1:D:249:GLU:HG3	1:D:471:TYR:HE2	1.66	0.58
1:B:329:THR:HG22	1:B:336:GLU:OE2	2.03	0.58
1:B:247:ALA:HB1	1:B:472:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:CYS:SG	1:A:382:TYR:HA	2.45	0.57
1:B:166:CYS:SG	1:B:382:TYR:HA	2.45	0.57
1:C:318[A]:ASN:HD22	1:C:343:LEU:CD2	2.18	0.57
1:B:153:GLY:C	1:B:154[A]:ASN:HD22	2.07	0.56
1:B:114[B]:MET:SD	1:B:119:LEU:CD2	2.86	0.56
1:D:318[A]:ASN:HD22	1:D:343:LEU:CD2	2.19	0.55
1:C:445:LEU:HB3	1:C:446:PRO:HD3	1.88	0.55
1:B:318[A]:ASN:HD22	1:B:343:LEU:CD2	2.20	0.55
1:A:249:GLU:HG3	1:A:471:TYR:HE2	1.72	0.55
2:B:1509:HMG:O1A	2:B:1509:HMG:O5A	2.26	0.53
1:B:154[B]:ASN:ND2	1:B:188[B]:ARG:NH2	2.56	0.53
1:A:318[A]:ASN:HD22	1:A:343:LEU:CD2	2.20	0.53
1:D:166:CYS:SG	1:D:382:TYR:HA	2.48	0.53
1:A:154[B]:ASN:ND2	1:A:188[B]:ARG:NH2	2.56	0.53
1:B:154[B]:ASN:HD21	1:B:188[B]:ARG:NH2	2.05	0.53
1:B:286:SER:OG	1:B:288:ARG:HG2	2.09	0.53
1:B:445:LEU:HB3	1:B:446:PRO:HD3	1.91	0.52
1:C:166:CYS:SG	1:C:382:TYR:HA	2.50	0.52
1:D:110:VAL:O	1:D:114[B]:MET:HG2	2.10	0.52
1:A:318[A]:ASN:CG	4:A:2234:HOH:O	2.47	0.52
1:A:154[B]:ASN:HD21	1:A:188[B]:ARG:NH2	2.08	0.52
1:A:447:LYS:HG2	1:B:373:TYR:CZ	2.45	0.52
1:B:318[A]:ASN:ND2	1:B:343:LEU:CD2	2.74	0.51
1:B:312:LEU:CD2	1:B:364:PHE:HA	2.40	0.51
1:D:445:LEU:HB3	1:D:446:PRO:HD3	1.92	0.51
1:C:475:ASN:ND2	1:C:497:GLU:HG3	2.25	0.51
1:C:318[A]:ASN:ND2	1:C:343:LEU:CD2	2.74	0.50
1:C:286:SER:OG	1:C:288:ARG:HG2	2.11	0.50
1:A:445:LEU:HB3	1:A:446:PRO:HD3	1.92	0.50
1:C:312:LEU:CD2	1:C:364:PHE:HA	2.41	0.50
1:A:312:LEU:CD2	1:A:364:PHE:HA	2.41	0.49
1:D:154:ASN:HB3	4:D:2122:HOH:O	2.11	0.49
1:D:312:LEU:CD2	1:D:364:PHE:HA	2.42	0.49
1:B:186:ASP:OD2	1:B:188[A]:ARG:NH2	2.44	0.49
1:A:318[A]:ASN:ND2	1:A:343:LEU:CD2	2.76	0.48
1:C:166:CYS:SG	2:C:1509:HMG:C5	3.01	0.48
1:D:114[B]:MET:SD	1:D:119:LEU:CD2	2.90	0.48
1:A:246:LEU:HD12	1:D:471:TYR:HE1	1.78	0.48
1:A:373:TYR:CZ	1:B:447:LYS:HG2	2.49	0.48
1:B:166:CYS:SG	2:B:1509:HMG:C5	3.02	0.48
1:B:310:LYS:HZ1	2:B:1509:HMG:P3B	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318[A]:ASN:ND2	4:C:2228:HOH:O	2.44	0.48
1:D:318[A]:ASN:ND2	1:D:343:LEU:CD2	2.77	0.48
1:D:166:CYS:SG	2:D:1509:HMG:C5	3.02	0.47
1:B:122:ASP:CA	1:B:154[A]:ASN:OD1	2.63	0.47
1:A:186:ASP:OD2	1:A:188[A]:ARG:NH2	2.44	0.47
1:D:497:GLU:HG2	1:D:498:GLN:CD	2.35	0.47
1:B:249:GLU:HG3	1:B:471:TYR:HE2	1.77	0.46
1:A:166:CYS:SG	2:A:1509:HMG:C5	3.04	0.46
1:B:113:LEU:HD23	1:B:191[B]:MET:SD	2.56	0.46
1:A:447:LYS:NZ	4:A:2314:HOH:O	2.33	0.46
1:C:113:LEU:HD23	1:C:191[B]:MET:SD	2.56	0.45
1:A:132:GLU:OE2	2:A:1509:HMG:O4	2.34	0.45
1:B:315:LEU:O	1:B:318[A]:ASN:HB2	2.17	0.45
1:A:274:ARG:NH2	1:A:318[B]:ASN:OD1	2.50	0.44
1:A:507:PRO:O	1:A:508:VAL:CB	2.64	0.44
1:B:471:TYR:HE1	1:C:246:LEU:HD12	1.82	0.44
1:D:247:ALA:O	1:D:472:HIS:NE2	2.44	0.44
1:B:508:VAL:HG23	4:B:2378:HOH:O	2.17	0.44
1:C:485:LEU:O	1:C:506:ARG:NH1	2.44	0.44
1:D:113:LEU:HD23	1:D:191[B]:MET:SD	2.57	0.44
1:D:132:GLU:OE2	2:D:1509:HMG:O4	2.36	0.44
1:A:400:GLN:HG3	4:A:2288:HOH:O	2.17	0.44
1:B:274:ARG:NH2	1:B:318[B]:ASN:OD1	2.51	0.44
1:C:487:PRO:HB3	1:C:508:VAL:HB	2.00	0.43
1:B:246:LEU:HD12	1:C:471:TYR:HE1	1.83	0.43
1:B:122:ASP:HA	1:B:154[A]:ASN:OD1	2.19	0.43
1:C:507:PRO:O	1:C:508:VAL:CB	2.65	0.43
1:B:110:VAL:O	1:B:114[B]:MET:HG2	2.17	0.43
1:D:98:VAL:HG11	1:D:470:PHE:HB2	2.00	0.43
1:A:240:ASP:HB2	1:A:258:SER:HA	2.00	0.43
1:C:240:ASP:HB2	1:C:258:SER:HA	2.01	0.43
1:B:240:ASP:HB2	1:B:258:SER:HA	2.00	0.43
1:C:416:LEU:C	1:C:416:LEU:HD12	2.39	0.43
1:D:416:LEU:C	1:D:416:LEU:HD12	2.38	0.43
1:A:246:LEU:HD12	1:D:471:TYR:CE1	2.54	0.43
1:C:98:VAL:HG11	1:C:470:PHE:HB2	2.00	0.43
1:D:241:PHE:HB3	1:D:414:SER:CB	2.48	0.43
1:D:447:LYS:HG3	4:D:2295:HOH:O	2.18	0.43
1:D:487:PRO:HB3	1:D:508:VAL:HB	2.01	0.43
1:B:241:PHE:HB3	1:B:414:SER:CB	2.49	0.43
1:D:186:ASP:OD2	1:D:188[A]:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASP:HB2	1:D:258:SER:HA	2.01	0.42
1:A:113:LEU:HD23	1:A:191[B]:MET:SD	2.60	0.42
1:B:507:PRO:C	1:B:508:VAL:HG13	2.39	0.42
1:B:471:TYR:CD1	1:B:471:TYR:C	2.93	0.42
1:A:485:LEU:O	1:A:506:ARG:NH1	2.45	0.42
1:D:247:ALA:HB1	1:D:472:HIS:CE1	2.54	0.42
1:A:98:VAL:HG11	1:A:470:PHE:HB2	2.01	0.42
1:B:415:GLY:N	1:B:416:LEU:HA	2.34	0.42
1:C:186:ASP:OD2	1:C:188:ARG:NH2	2.46	0.42
1:A:416:LEU:HD12	1:A:416:LEU:C	2.39	0.42
1:A:315:LEU:O	1:A:318[A]:ASN:HB2	2.20	0.41
1:B:416:LEU:HD12	1:B:416:LEU:C	2.39	0.41
1:B:487:PRO:HB2	1:B:508:VAL:HG22	2.00	0.41
1:A:471:TYR:HE1	1:D:246:LEU:HD12	1.85	0.41
1:A:487:PRO:HB3	1:A:508:VAL:HB	2.02	0.41
1:D:274:ARG:NH2	1:D:318[B]:ASN:OD1	2.54	0.41
1:B:98:VAL:HG11	1:B:470:PHE:HB2	2.01	0.41
1:B:247:ALA:HB1	1:B:472:HIS:NE2	2.35	0.41
1:A:310:LYS:HZ1	2:A:1509:HMG:P3B	2.44	0.41
1:C:315:LEU:O	1:C:318[A]:ASN:HB2	2.20	0.41
1:D:415:GLY:N	1:D:416:LEU:HA	2.35	0.41
1:D:506:ARG:HG2	1:D:507:PRO:HD2	2.03	0.41
1:A:241:PHE:HB3	1:A:414:SER:CB	2.50	0.41
1:C:415:GLY:N	1:C:416:LEU:HA	2.36	0.41
1:D:315:LEU:O	1:D:318[A]:ASN:HB2	2.21	0.41
1:B:247:ALA:O	1:B:472:HIS:NE2	2.54	0.41
1:C:241:PHE:HB3	1:C:414:SER:CB	2.51	0.41
1:D:114[B]:MET:CE	1:D:119:LEU:HD23	2.51	0.41
1:D:475:ASN:OD1	1:D:494:ARG:NH2	2.53	0.41
1:A:313:ALA:HB1	1:A:356:LEU:HB3	2.03	0.41
1:C:506:ARG:HG2	1:C:507:PRO:HD2	2.03	0.40
1:A:287:ASP:HB2	4:A:2213:HOH:O	2.21	0.40
1:A:475:ASN:OD1	1:A:494:ARG:NH2	2.54	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	466/460 (101%)	459 (98%)	6 (1%)	1 (0%)	47	30
1	B	467/460 (102%)	459 (98%)	7 (2%)	1 (0%)	47	30
1	C	465/460 (101%)	459 (99%)	5 (1%)	1 (0%)	47	30
1	D	471/460 (102%)	464 (98%)	6 (1%)	1 (0%)	47	30
All	All	1869/1840 (102%)	1841 (98%)	24 (1%)	4 (0%)	47	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ILE
1	B	160	ILE
1	C	160	ILE
1	D	160	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	384/391 (98%)	377 (98%)	7 (2%)	59	43
1	B	388/391 (99%)	379 (98%)	9 (2%)	50	33
1	C	382/391 (98%)	374 (98%)	8 (2%)	53	36
1	D	390/391 (100%)	381 (98%)	9 (2%)	50	33
All	All	1544/1564 (99%)	1511 (98%)	33 (2%)	57	36

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	PHE
1	A	318[A]	ASN
1	A	318[B]	ASN
1	A	325	SER
1	A	471	TYR
1	A	494	ARG
1	A	499	HIS
1	B	79	VAL
1	B	241	PHE
1	B	318[A]	ASN
1	B	318[B]	ASN
1	B	325	SER
1	B	471	TYR
1	B	494	ARG
1	B	499	HIS
1	B	508	VAL
1	C	241	PHE
1	C	318[A]	ASN
1	C	318[B]	ASN
1	C	325	SER
1	C	400	GLN
1	C	471	TYR
1	C	494	ARG
1	C	499	HIS
1	D	241	PHE
1	D	318[A]	ASN
1	D	318[B]	ASN
1	D	325	SER
1	D	400	GLN
1	D	471	TYR
1	D	473	LYS
1	D	494	ARG
1	D	499	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	396	HIS
1	A	483	ASN
1	B	78	ASN

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Mol	Chain	Res	Type
1	B	396	HIS
1	B	483	ASN
1	D	78	ASN
1	D	154	ASN
1	D	483	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	HMG	C	1509	-	54,60,60	2.43	13 (24%)	68,90,90	1.71	11 (16%)
2	HMG	A	1509	-	54,60,60	2.38	12 (22%)	68,90,90	1.75	9 (13%)
3	GOL	A	1510	-	5,5,5	0.35	0	5,5,5	0.39	0
2	HMG	D	1509	-	54,60,60	2.45	12 (22%)	68,90,90	1.74	10 (14%)
2	HMG	B	1509	-	54,60,60	2.40	13 (24%)	68,90,90	1.75	11 (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
2	HMG	C	1509	-	-	4/56/77/77	0/3/3/3
2	HMG	A	1509	-	-	4/56/77/77	0/3/3/3
3	GOL	A	1510	-	-	4/4/4/4	-
2	HMG	D	1509	-	-	3/56/77/77	0/3/3/3
2	HMG	B	1509	-	-	2/56/77/77	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1509	HMG	C2A-N3A	9.56	1.46	1.32
2	A	1509	HMG	C2A-N3A	9.41	1.46	1.32
2	C	1509	HMG	C2A-N3A	9.33	1.46	1.32
2	B	1509	HMG	C2A-N3A	9.23	1.46	1.32
2	C	1509	HMG	C9P-N8P	5.66	1.46	1.33
2	D	1509	HMG	C9P-N8P	5.58	1.46	1.33
2	B	1509	HMG	C9P-N8P	5.39	1.46	1.33
2	A	1509	HMG	C9P-N8P	5.37	1.46	1.33
2	D	1509	HMG	C8A-N7A	5.26	1.44	1.34
2	C	1509	HMG	C8A-N7A	5.21	1.44	1.34
2	B	1509	HMG	C8A-N7A	5.13	1.44	1.34
2	D	1509	HMG	C2A-N1A	5.08	1.43	1.33
2	A	1509	HMG	C8A-N7A	5.06	1.44	1.34
2	A	1509	HMG	C2A-N1A	5.06	1.42	1.33
2	C	1509	HMG	C2A-N1A	4.99	1.42	1.33
2	B	1509	HMG	C2A-N1A	4.91	1.42	1.33
2	C	1509	HMG	C5P-N4P	4.80	1.44	1.33
2	A	1509	HMG	C5P-N4P	4.69	1.44	1.33
2	A	1509	HMG	O4B-C1B	4.60	1.46	1.40
2	D	1509	HMG	C5P-N4P	4.60	1.44	1.33
2	B	1509	HMG	O4B-C1B	4.56	1.46	1.40
2	B	1509	HMG	C5P-N4P	4.55	1.44	1.33
2	D	1509	HMG	O4B-C1B	4.49	1.46	1.40
2	C	1509	HMG	O4B-C1B	4.45	1.46	1.40
2	B	1509	HMG	C4A-N3A	3.57	1.40	1.35
2	C	1509	HMG	O7-C3	-3.51	1.39	1.44
2	D	1509	HMG	O7-C3	-3.49	1.39	1.44
2	A	1509	HMG	C4A-N3A	3.34	1.40	1.35
2	D	1509	HMG	C4A-N3A	3.31	1.40	1.35
2	D	1509	HMG	O4B-C4B	3.29	1.52	1.45
2	C	1509	HMG	C4A-N3A	3.29	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1509	HMG	O7-C3	-3.08	1.40	1.44
2	C	1509	HMG	O4B-C4B	3.02	1.51	1.45
2	B	1509	HMG	O4B-C4B	3.00	1.51	1.45
2	A	1509	HMG	O4B-C4B	2.90	1.51	1.45
2	B	1509	HMG	C6A-N6A	2.78	1.44	1.34
2	C	1509	HMG	C6A-N6A	2.74	1.43	1.34
2	D	1509	HMG	C6A-N6A	2.74	1.43	1.34
2	A	1509	HMG	C6A-N6A	2.69	1.43	1.34
2	C	1509	HMG	C6A-C5A	2.63	1.53	1.43
2	D	1509	HMG	C6A-C5A	2.57	1.53	1.43
2	A	1509	HMG	O7-C3	-2.55	1.40	1.44
2	A	1509	HMG	C6A-C5A	2.51	1.52	1.43
2	B	1509	HMG	C6A-C5A	2.50	1.52	1.43
2	C	1509	HMG	O4-C5	2.21	1.38	1.30
2	C	1509	HMG	P3B-O7A	2.09	1.57	1.50
2	B	1509	HMG	O4-C5	2.07	1.37	1.30
2	D	1509	HMG	C3B-C4B	2.05	1.58	1.52
2	B	1509	HMG	C4-C3	2.04	1.57	1.54
2	A	1509	HMG	O2B-C2B	-2.03	1.37	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1509	HMG	C6-C3-C4	-7.19	102.51	111.30
2	A	1509	HMG	C6-C3-C4	-7.17	102.54	111.30
2	B	1509	HMG	N3A-C2A-N1A	-6.61	119.70	128.67
2	B	1509	HMG	C6-C3-C4	-6.53	103.32	111.30
2	A	1509	HMG	N3A-C2A-N1A	-6.50	119.84	128.67
2	C	1509	HMG	N3A-C2A-N1A	-6.40	119.98	128.67
2	D	1509	HMG	N3A-C2A-N1A	-6.27	120.17	128.67
2	C	1509	HMG	C6-C3-C4	-6.14	103.80	111.30
2	D	1509	HMG	C4B-O4B-C1B	-4.44	105.86	109.92
2	A	1509	HMG	C4B-O4B-C1B	-4.43	105.87	109.92
2	C	1509	HMG	C4B-O4B-C1B	-3.91	106.35	109.92
2	A	1509	HMG	C6-C3-C2	3.70	115.82	111.30
2	D	1509	HMG	C6-C3-C2	3.61	115.70	111.30
2	A	1509	HMG	O2B-C2B-C3B	3.47	120.90	111.19
2	C	1509	HMG	O2B-C2B-C3B	3.45	120.85	111.19
2	C	1509	HMG	O2-C1-S1P	-3.40	118.35	122.68
2	B	1509	HMG	O2B-C2B-C3B	3.37	120.62	111.19
2	B	1509	HMG	C4B-O4B-C1B	-3.37	106.84	109.92
2	B	1509	HMG	C6-C3-C2	3.23	115.25	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1509	HMG	O2-C1-S1P	-3.22	118.58	122.68
2	D	1509	HMG	O2B-C2B-C3B	3.12	119.93	111.19
2	A	1509	HMG	O2-C1-S1P	-3.07	118.77	122.68
2	C	1509	HMG	C6-C3-C2	2.83	114.76	111.30
2	C	1509	HMG	C2-C1-S1P	2.80	117.09	113.56
2	B	1509	HMG	O6A-CCP-CBP	2.75	114.96	110.55
2	C	1509	HMG	O4-C5-C4	2.49	122.23	114.35
2	D	1509	HMG	C7P-N8P-C9P	-2.28	118.46	122.55
2	B	1509	HMG	O4-C5-C4	2.27	121.54	114.35
2	D	1509	HMG	O4B-C4B-C5B	2.22	116.46	109.33
2	A	1509	HMG	O4B-C4B-C5B	2.17	116.27	109.33
2	A	1509	HMG	O7-C3-C6	2.16	113.32	108.09
2	B	1509	HMG	C7P-C6P-C5P	2.15	115.98	112.39
2	C	1509	HMG	O3B-C3B-C4B	2.15	117.61	110.03
2	A	1509	HMG	O3B-C3B-C4B	2.14	117.57	110.03
2	D	1509	HMG	O2-C1-S1P	-2.14	119.96	122.68
2	B	1509	HMG	O7-C3-C6	2.11	113.20	108.09
2	D	1509	HMG	C7P-C6P-C5P	2.09	115.87	112.39
2	C	1509	HMG	CDP-CBP-CCP	2.08	111.65	108.22
2	D	1509	HMG	CDP-CBP-CCP	2.04	111.59	108.22
2	C	1509	HMG	O4B-C4B-C5B	2.04	115.86	109.33
2	B	1509	HMG	O3B-C3B-C2B	2.01	118.90	111.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1509	HMG	C1-C2-C3-O7
2	B	1509	HMG	C1-C2-C3-O7
2	C	1509	HMG	C1-C2-C3-O7
2	D	1509	HMG	C1-C2-C3-O7
3	A	1510	GOL	O1-C1-C2-C3
3	A	1510	GOL	C1-C2-C3-O3
3	A	1510	GOL	O2-C2-C3-O3
2	D	1509	HMG	O4B-C4B-C5B-O5B
3	A	1510	GOL	O1-C1-C2-O2
2	D	1509	HMG	C3B-C4B-C5B-O5B
2	A	1509	HMG	O4B-C4B-C5B-O5B
2	A	1509	HMG	C3B-C4B-C5B-O5B
2	C	1509	HMG	C3-C4-C5-O3
2	C	1509	HMG	O4B-C4B-C5B-O5B
2	B	1509	HMG	C3-C4-C5-O3

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Mol	Chain	Res	Type	Atoms
2	C	1509	HMG	C1-C2-C3-C6
2	A	1509	HMG	P1A-O3A-P2A-O4A

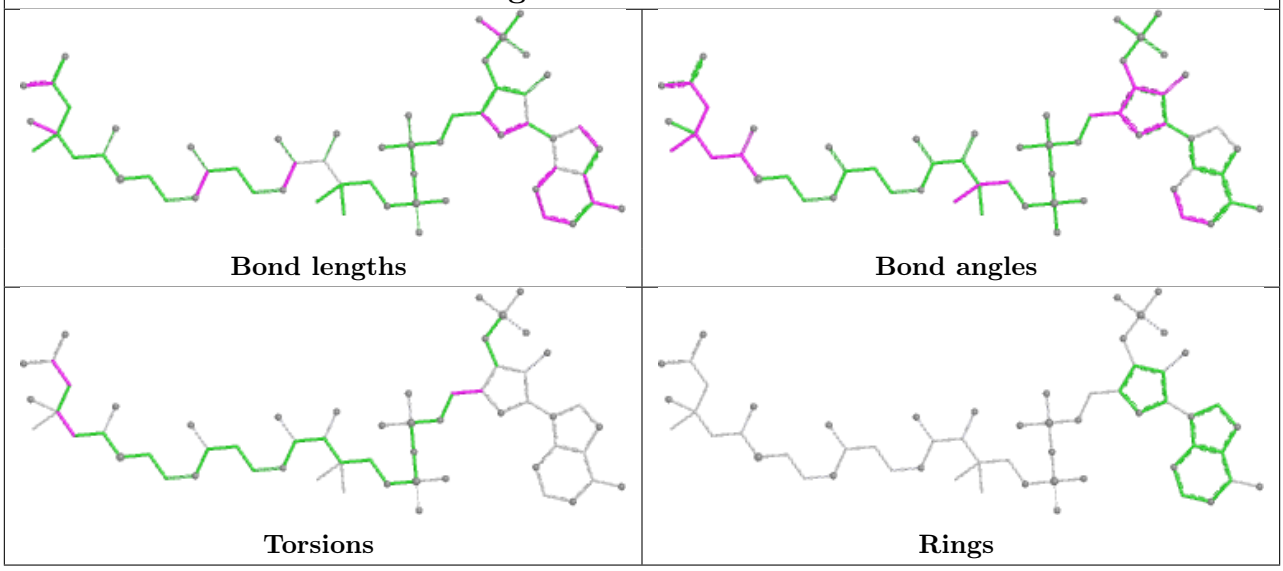
There are no ring outliers.

4 monomers are involved in 9 short contacts:

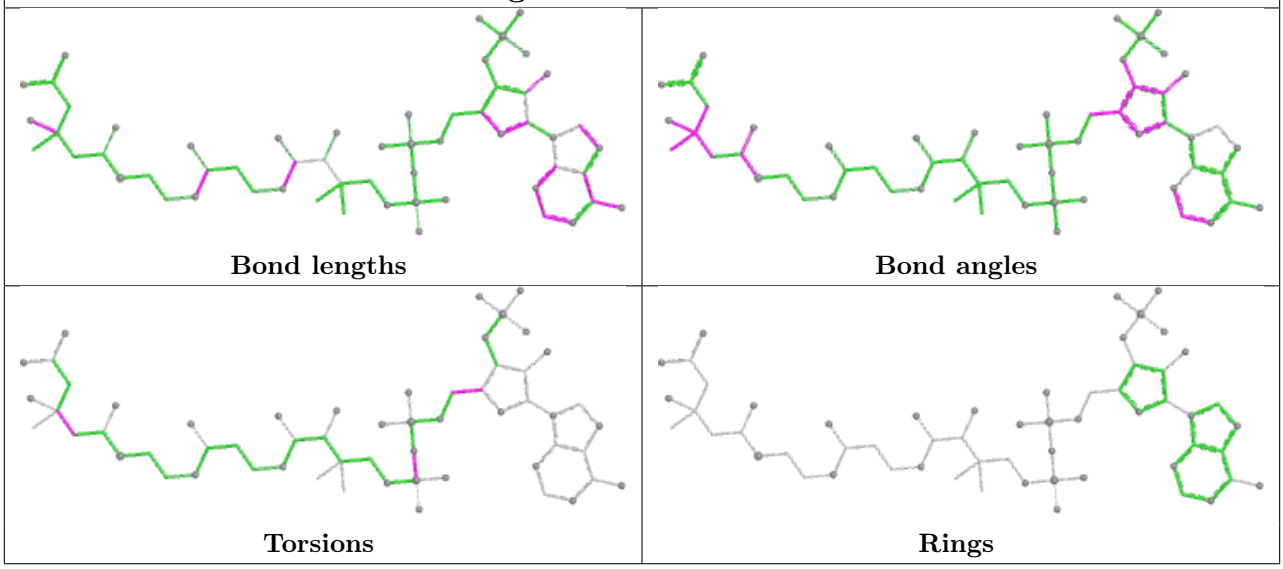
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1509	HMG	1	0
2	A	1509	HMG	3	0
2	D	1509	HMG	2	0
2	B	1509	HMG	3	0

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

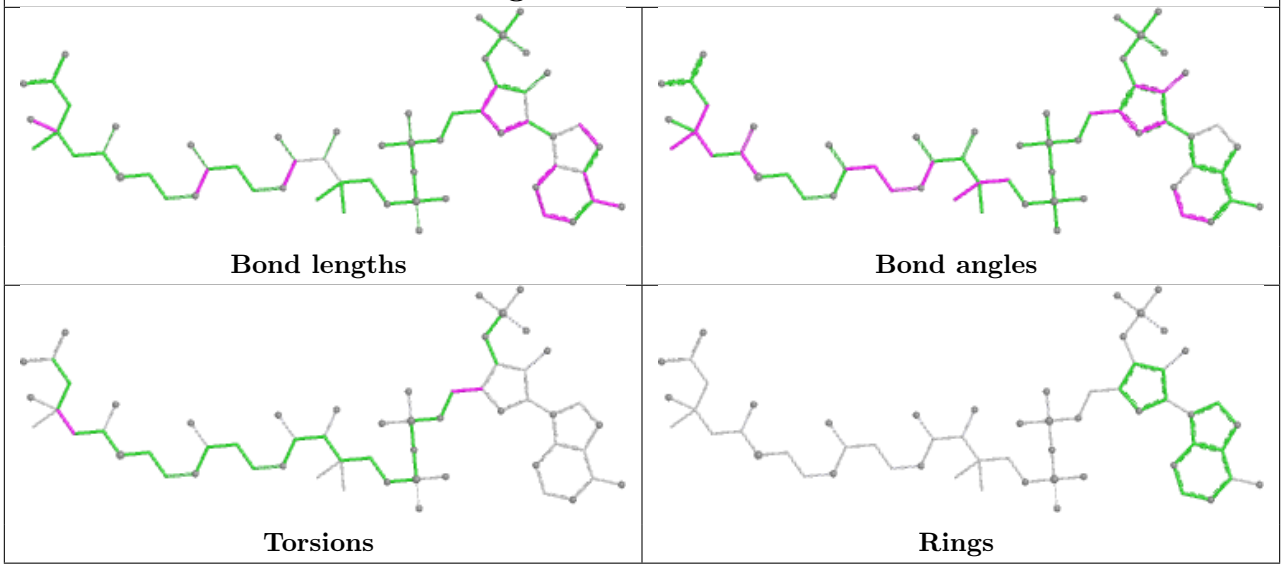
Ligand HMG C 1509

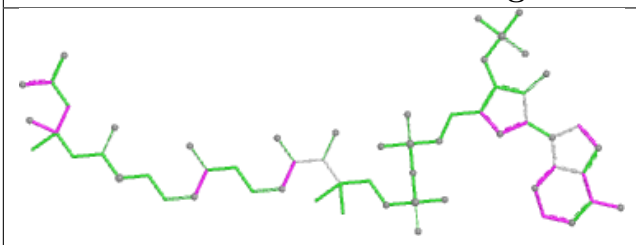
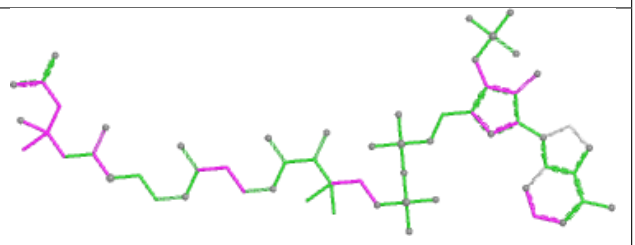
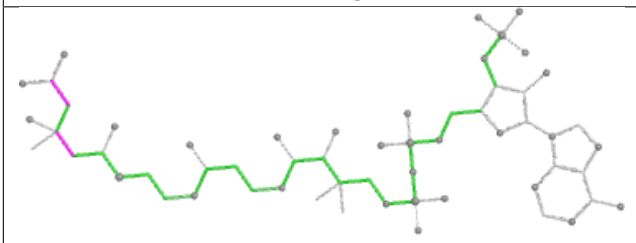
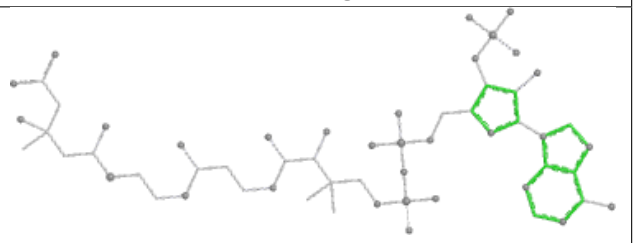


Ligand HMG A 1509



Ligand HMG D 1509



Ligand HMG B 1509	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	460/460 (100%)	-0.36	11 (2%)	59	63	7, 17, 39, 62	0
1	B	460/460 (100%)	-0.30	11 (2%)	59	63	8, 17, 39, 70	0
1	C	460/460 (100%)	-0.32	10 (2%)	62	66	8, 17, 39, 62	0
1	D	460/460 (100%)	-0.26	15 (3%)	46	51	8, 17, 40, 62	0
All	All	1840/1840 (100%)	-0.31	47 (2%)	56	60	7, 17, 40, 70	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	471	TYR	8.2
1	B	325	SER	4.5
1	A	329	THR	4.2
1	A	508	VAL	4.2
1	A	471	TYR	4.1
1	D	329	THR	3.8
1	D	325	SER	3.8
1	B	284	ALA	3.8
1	B	329	THR	3.8
1	B	326	ASP	3.8
1	C	49	SER	3.7
1	B	327	THR	3.5
1	C	287	ASP	3.3
1	B	508	VAL	3.3
1	D	470	PHE	3.2
1	D	471	TYR	3.2
1	C	325	SER	3.1
1	A	331	LEU	3.1
1	A	325	SER	3.0
1	B	471	TYR	3.0
1	C	329	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	347	TYR	3.0
1	D	285	GLY	2.9
1	B	283	GLN	2.9
1	B	285	GLY	2.8
1	A	49	SER	2.8
1	C	347	TYR	2.7
1	D	284	ALA	2.6
1	A	347	TYR	2.6
1	D	476	PHE	2.6
1	D	286	SER	2.5
1	D	283	GLN	2.5
1	B	287	ASP	2.5
1	D	288[A]	ARG	2.4
1	D	326	ASP	2.4
1	C	431	PRO	2.3
1	C	430	ALA	2.3
1	D	49	SER	2.2
1	D	287	ASP	2.2
1	C	285	GLY	2.2
1	D	508	VAL	2.2
1	A	330	SER	2.2
1	A	326	ASP	2.1
1	A	327	THR	2.1
1	A	287	ASP	2.1
1	D	483	ASN	2.1
1	C	482	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

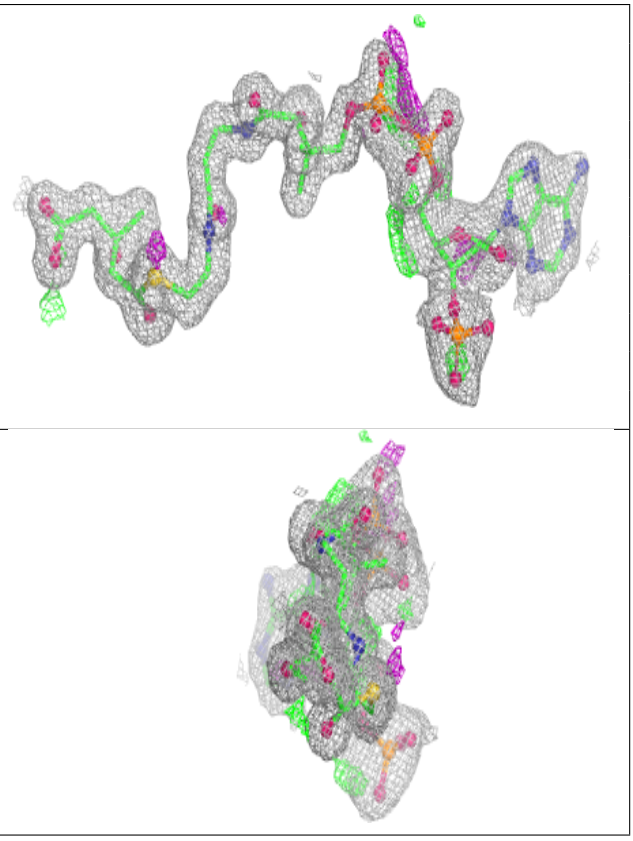
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1510	6/6	0.80	0.17	55,58,60,63	0
2	HMG	B	1509	58/58	0.93	0.11	9,28,63,79	0
2	HMG	A	1509	58/58	0.93	0.11	10,26,57,82	0
2	HMG	D	1509	58/58	0.94	0.12	11,31,59,75	0
2	HMG	C	1509	58/58	0.94	0.10	10,28,66,71	0

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

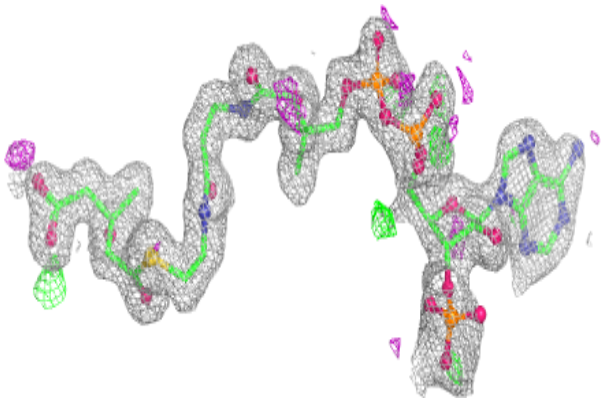
Electron density around HMG B 1509:

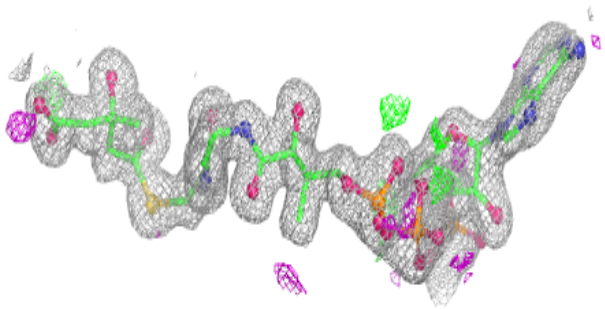
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

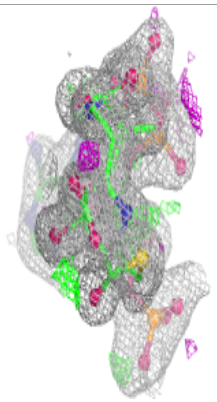


Electron density around HMG A 1509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

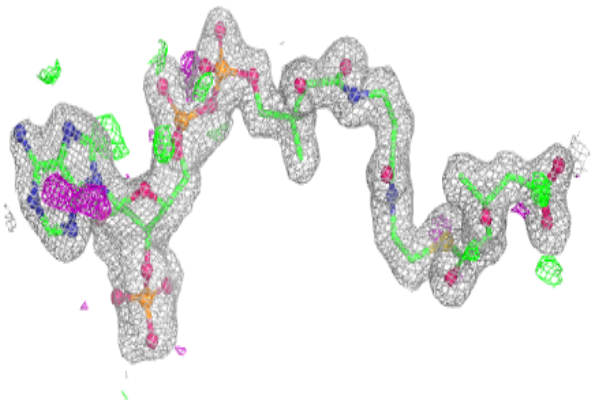


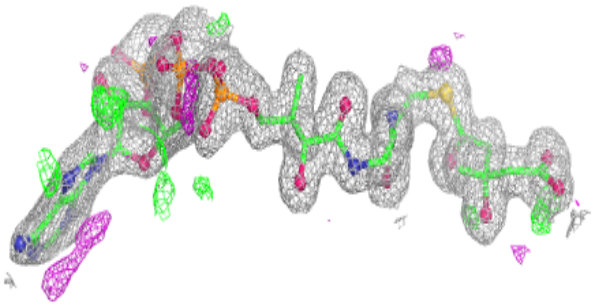


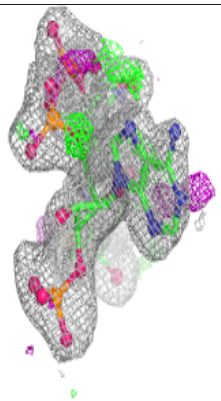


Electron density around HMG D 1509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

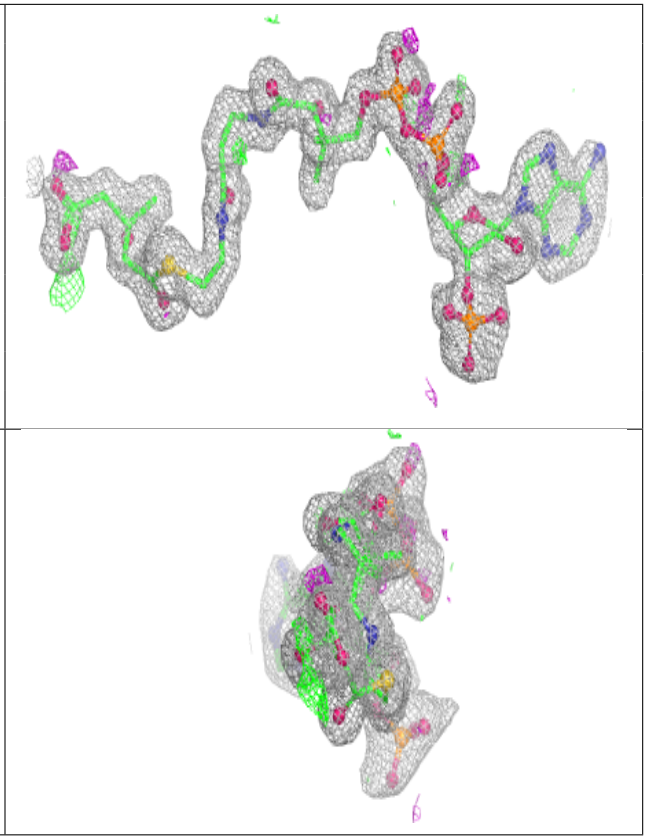






Electron density around HMG C 1509:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.