



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:04 am BST

PDB ID : 1E7C  
Title : HUMAN SERUM ALBUMIN COMPLEXED WITH MYRISTIC ACID and  
the general anesthetic halothane  
Authors : Bhattacharya, A.A.; Curry, S.; Franks, N.P.  
Deposited on : 2000-08-26  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

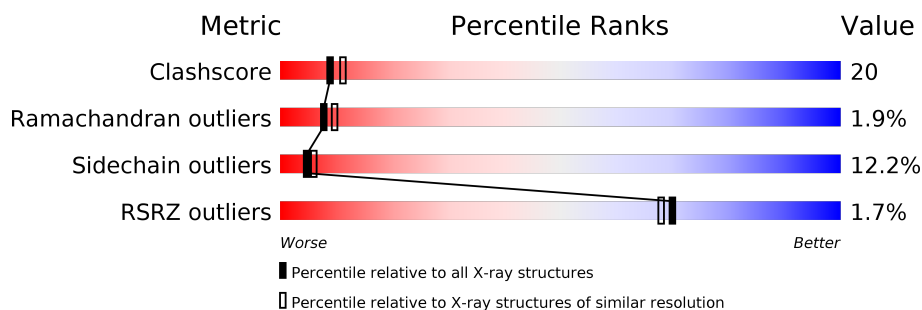
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ . 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	585	

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
3	HLT	A	4001	-	-	X	-
3	HLT	A	4004	-	-	X	-
3	HLT	A	4006	-	-	X	-

## 2 Entry composition [i](#)

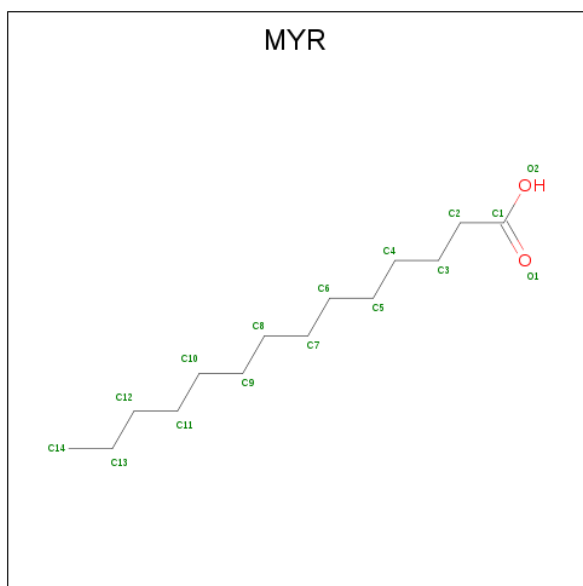
There are 4 unique types of molecules in this entry. The entry contains 4635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM ALBUMIN.

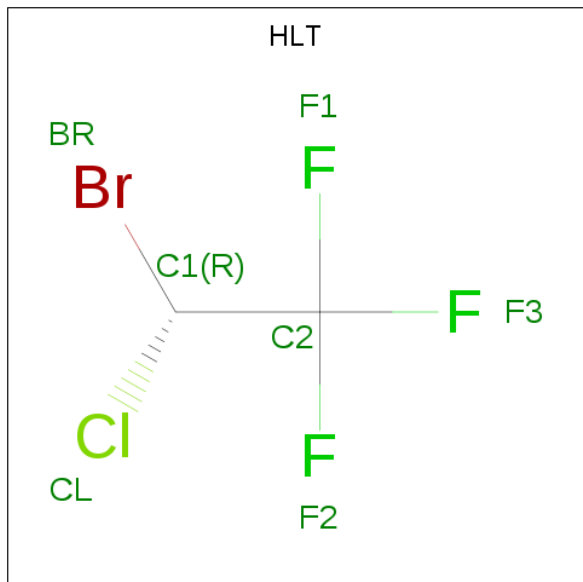
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4477	2835	757	844	41			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			15	13	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is 2-BROMO-2-CHLORO-1,1,1-TRIFLUOROETHANE (three-letter code: HLT) (formula:  $C_2HBrClF_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
3	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
3	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
3	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
3	A	1	Total	Br	C	Cl	F	0	0
			7	1	2	1	3		
3	A	1	Total	Br	C	Cl	F	0	1
			14	2	4	2	6		

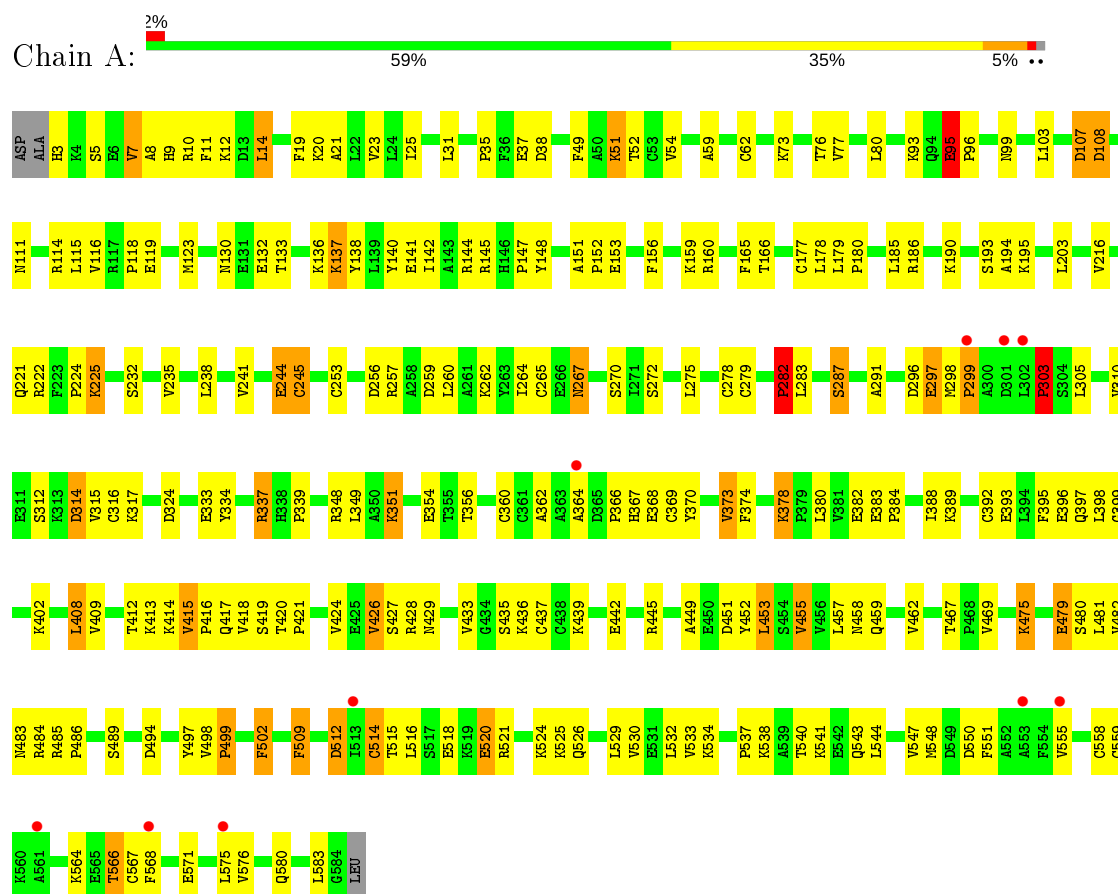
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		

### 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 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: SERUM ALBUMIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.91Å 39.08Å 96.69Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	47.00 – 2.40 46.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.00-2.40) 98.9 (46.02-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.232 , 0.282 0.217 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, HLT

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	0.38	0/4566	0.60	3/6187 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	245	CYS	N-CA-CB	5.77	120.99	110.60
1	A	244	GLU	C-N-CA	5.28	134.90	121.70
1	A	282	PRO	CA-N-CD	-5.18	104.25	111.50

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	4477	0	4275	179	0
2	A	70	0	103	3	0
3	A	56	0	0	8	0
4	A	32	0	0	7	0
All	All	4635	0	4378	181	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 20.

All (181) 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:A:225:LYS:HG3	1:A:299:PRO:HD3	1.41	1.03
1:A:195:LYS:NZ	1:A:451:ASP:OD1	1.90	1.03
1:A:559:CYS:SG	1:A:568:PHE:CZ	2.58	0.96
1:A:111:ASN:HB2	4:A:2010:HOH:O	1.69	0.92
1:A:195:LYS:HZ3	1:A:451:ASP:CG	1.74	0.91
1:A:225:LYS:HG3	1:A:299:PRO:CD	2.03	0.88
1:A:222:ARG:HD2	3:A:4006:HLT:CL	2.11	0.87
1:A:303:PRO:O	1:A:337:ARG:NH1	2.08	0.87
1:A:559:CYS:SG	1:A:568:PHE:HZ	1.98	0.83
1:A:559:CYS:SG	1:A:568:PHE:CE2	2.73	0.82
1:A:424:VAL:O	1:A:428:ARG:HG3	1.81	0.80
1:A:521:ARG:O	1:A:525:LYS:HG3	1.82	0.80
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.63	0.79
1:A:114:ARG:HH21	1:A:116:VAL:HG12	1.46	0.78
1:A:257:ARG:HH21	1:A:287:SER:HB2	1.49	0.76
1:A:479:GLU:HG3	1:A:480:SER:H	1.51	0.75
1:A:12:LYS:HE2	1:A:54:VAL:HG13	1.68	0.75
1:A:222:ARG:NH1	1:A:291:ALA:O	2.19	0.73
1:A:225:LYS:HG3	1:A:299:PRO:CG	2.18	0.72
1:A:222:ARG:HG3	4:A:2017:HOH:O	1.88	0.72
1:A:195:LYS:CE	1:A:451:ASP:OD1	2.40	0.70
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.74	0.70
1:A:10:ARG:O	1:A:14:LEU:HB2	1.92	0.69
1:A:195:LYS:NZ	1:A:451:ASP:CG	2.41	0.69
1:A:530:VAL:HG12	1:A:534:LYS:HE3	1.76	0.68
1:A:567:CYS:O	1:A:571:GLU:HB2	1.93	0.68
1:A:114:ARG:NH2	1:A:116:VAL:HG12	2.09	0.68
1:A:138:TYR:O	1:A:142:ILE:HG12	1.94	0.67
1:A:479:GLU:HG2	1:A:483:ASN:HB2	1.75	0.67
1:A:133:THR:O	1:A:137:LYS:HB2	1.94	0.66
1:A:136:LYS:HE2	3:A:4008[B]:HLT:CL	2.33	0.65
1:A:558:CYS:HB3	1:A:568:PHE:CD2	2.31	0.65
1:A:119:GLU:HB3	4:A:2011:HOH:O	1.96	0.64
1:A:221:GLN:HG2	1:A:339:PRO:HA	1.80	0.63
3:A:4001:HLT:CL	3:A:4002:HLT:F1	2.45	0.62
1:A:449:ALA:O	1:A:453:LEU:HB2	1.99	0.62
1:A:398:LEU:HB3	1:A:402:LYS:HB3	1.81	0.62
1:A:225:LYS:HG3	1:A:299:PRO:HG3	1.82	0.61
1:A:118:PRO:HD2	1:A:123:MET:CE	2.31	0.61
1:A:21:ALA:O	1:A:25:ILE:HG13	2.01	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASN:O	1:A:462:VAL:HG23	2.00	0.61
1:A:222:ARG:CG	4:A:2017:HOH:O	2.47	0.60
1:A:520:GLU:HA	1:A:520:GLU:OE1	2.01	0.60
1:A:349:LEU:HD23	1:A:380:LEU:HD23	1.83	0.60
1:A:107:ASP:O	1:A:147:PRO:HG2	2.02	0.60
1:A:356:THR:HG21	1:A:373:VAL:CG2	2.32	0.60
1:A:267:ASN:N	1:A:267:ASN:HD22	2.00	0.59
1:A:366:PRO:C	1:A:368:GLU:H	2.06	0.59
1:A:225:LYS:HD2	1:A:297:GLU:O	2.02	0.59
1:A:195:LYS:NZ	1:A:451:ASP:OD2	2.36	0.59
1:A:3:HIS:NE2	1:A:9:HIS:CE1	2.71	0.58
1:A:73:LYS:O	1:A:76:THR:HB	2.04	0.58
1:A:395:PHE:CZ	1:A:435:SER:HB3	2.38	0.58
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.44	0.57
1:A:419:SER:OG	1:A:421:PRO:HD2	2.04	0.57
1:A:550:ASP:HB3	1:A:575:LEU:HD11	1.87	0.57
1:A:452:TYR:O	1:A:455:VAL:HG23	2.05	0.56
1:A:244:GLU:HG3	1:A:256:ASP:OD2	2.04	0.56
1:A:409:VAL:O	1:A:413:LYS:HG3	2.05	0.56
1:A:195:LYS:HE2	1:A:451:ASP:OD1	2.04	0.56
1:A:159:LYS:HG2	3:A:4008[A]:HLT:BR	2.62	0.55
1:A:224:PRO:HG2	1:A:298:MET:HA	1.89	0.55
1:A:8:ALA:O	1:A:12:LYS:HG3	2.06	0.55
1:A:475:LYS:HE2	1:A:475:LYS:O	2.07	0.54
3:A:4005:HLT:F3	3:A:4006:HLT:BR	2.70	0.54
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.89	0.54
1:A:245:CYS:HA	1:A:253:CYS:HB2	1.90	0.54
1:A:296:ASP:OD1	1:A:297:GLU:N	2.41	0.54
1:A:530:VAL:CG1	1:A:534:LYS:HE3	2.38	0.53
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.89	0.52
1:A:393:GLU:OE1	1:A:393:GLU:HA	2.08	0.52
1:A:366:PRO:O	1:A:368:GLU:N	2.42	0.52
1:A:356:THR:HG21	1:A:373:VAL:HG23	1.92	0.52
1:A:479:GLU:HG3	1:A:480:SER:N	2.20	0.52
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.91	0.52
1:A:558:CYS:HB3	1:A:568:PHE:CE2	2.45	0.52
1:A:373:VAL:HG12	1:A:374:PHE:N	2.25	0.52
1:A:540:THR:HG22	1:A:541:LYS:N	2.25	0.52
1:A:324:ASP:HB3	3:A:4001:HLT:F1	2.00	0.52
1:A:225:LYS:CG	1:A:299:PRO:HG3	2.39	0.51
1:A:244:GLU:CG	1:A:256:ASP:OD2	2.59	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:O	1:A:393:GLU:HG2	2.09	0.51
1:A:509:PHE:N	1:A:509:PHE:CD1	2.78	0.51
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.93	0.51
1:A:559:CYS:SG	1:A:568:PHE:HE2	2.28	0.51
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.92	0.51
1:A:408:LEU:HD13	1:A:427:SER:CB	2.41	0.51
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.44	0.51
1:A:551:PHE:O	1:A:555:VAL:HG23	2.12	0.50
1:A:480:SER:C	1:A:482:VAL:H	2.15	0.50
1:A:224:PRO:CG	1:A:298:MET:HA	2.41	0.50
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.40	0.49
1:A:115:LEU:HD13	1:A:145:ARG:CZ	2.42	0.49
1:A:415:VAL:HB	1:A:418:VAL:HG23	1.94	0.49
1:A:420:THR:N	1:A:421:PRO:HD2	2.28	0.49
1:A:426:VAL:HG12	1:A:427:SER:N	2.27	0.49
1:A:547:VAL:HG21	1:A:583:LEU:HD21	1.94	0.49
1:A:351:LYS:HE3	1:A:354:GLU:OE1	2.12	0.48
1:A:118:PRO:HD2	1:A:123:MET:HE3	1.94	0.48
1:A:19:PHE:O	1:A:23:VAL:HG23	2.12	0.48
1:A:35:PRO:O	1:A:38:ASP:HB2	2.14	0.48
1:A:393:GLU:O	1:A:397:GLN:HG3	2.13	0.48
1:A:186:ARG:O	1:A:190:LYS:HG3	2.13	0.48
1:A:366:PRO:C	1:A:368:GLU:N	2.67	0.48
1:A:49:PHE:O	1:A:52:THR:HB	2.14	0.48
1:A:378:LYS:O	1:A:382:GLU:HG3	2.14	0.48
1:A:429:ASN:O	1:A:433:VAL:HG23	2.13	0.47
1:A:516:LEU:O	1:A:521:ARG:HD2	2.14	0.47
1:A:123:MET:HE1	2:A:1001:MYR:H62	1.96	0.47
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.49	0.47
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.45	0.47
1:A:540:THR:HG22	1:A:541:LYS:H	1.79	0.47
1:A:576:VAL:O	1:A:580:GLN:HB2	2.15	0.47
1:A:566:THR:HG22	1:A:567:CYS:N	2.29	0.47
1:A:259:ASP:O	1:A:262:LYS:HG2	2.15	0.47
1:A:399:GLY:HA3	4:A:2028:HOH:O	2.14	0.47
1:A:314:ASP:HB3	1:A:317:LYS:HB3	1.98	0.46
1:A:310:VAL:O	1:A:370:TYR:HE1	1.98	0.46
1:A:360:CYS:C	1:A:362:ALA:H	2.18	0.46
1:A:77:VAL:O	1:A:80:LEU:HB2	2.14	0.46
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.98	0.46
1:A:216:VAL:CG2	1:A:235:VAL:HG21	2.46	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:CYS:SG	1:A:279:CYS:CB	3.04	0.46
1:A:275:LEU:O	1:A:279:CYS:SG	2.61	0.46
1:A:499:PRO:HG3	1:A:537:PRO:HG2	1.98	0.46
1:A:118:PRO:HD2	1:A:123:MET:HE2	1.96	0.46
1:A:348:ARG:HG3	1:A:482:VAL:HG13	1.97	0.45
1:A:11:PHE:CZ	1:A:51:LYS:HD2	2.52	0.45
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.52	0.45
1:A:272:SER:OG	1:A:296:ASP:HB2	2.17	0.45
1:A:360:CYS:HB3	1:A:369:CYS:HB3	1.90	0.45
1:A:216:VAL:HG21	3:A:4004:HLT:F2	2.06	0.45
1:A:260:LEU:O	1:A:264:ILE:HG13	2.17	0.45
1:A:298:MET:O	1:A:299:PRO:C	2.55	0.45
1:A:530:VAL:O	1:A:534:LYS:HG3	2.17	0.45
1:A:532:LEU:HD12	1:A:532:LEU:O	2.17	0.44
1:A:548:MET:HG2	2:A:1005:MYR:H52	1.99	0.44
1:A:95:GLU:OE2	1:A:99:ASN:HB2	2.17	0.44
1:A:130:ASN:OD1	1:A:133:THR:HG23	2.18	0.44
1:A:137:LYS:O	1:A:141:GLU:HG2	2.18	0.44
1:A:514:CYS:HB3	1:A:559:CYS:HB3	1.68	0.44
1:A:529:LEU:O	1:A:533:VAL:HG23	2.18	0.44
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.18	0.43
1:A:194:ALA:CB	1:A:455:VAL:HG12	2.48	0.43
1:A:156:PHE:CZ	1:A:160:ARG:HD2	2.53	0.43
1:A:384:PRO:O	1:A:388:ILE:HG12	2.18	0.43
1:A:392:CYS:O	1:A:396:GLU:HG3	2.19	0.43
1:A:412:THR:HG21	1:A:533:VAL:HB	2.00	0.43
1:A:420:THR:O	1:A:424:VAL:HG23	2.18	0.43
1:A:20:LYS:NZ	4:A:2001:HOH:O	2.28	0.43
1:A:315:VAL:HG11	1:A:370:TYR:CZ	2.54	0.43
1:A:480:SER:C	1:A:482:VAL:N	2.72	0.43
1:A:437:CYS:C	1:A:439:LYS:H	2.22	0.43
1:A:512:ASP:OD1	1:A:512:ASP:N	2.51	0.43
1:A:408:LEU:CD2	1:A:526:GLN:HG2	2.49	0.43
1:A:95:GLU:O	1:A:95:GLU:OE2	2.37	0.43
1:A:547:VAL:CG2	1:A:583:LEU:HD21	2.49	0.43
1:A:224:PRO:HD2	1:A:296:ASP:HB3	2.00	0.42
1:A:225:LYS:CG	1:A:299:PRO:HD3	2.29	0.42
1:A:512:ASP:O	1:A:515:THR:HG22	2.19	0.42
1:A:194:ALA:HB1	1:A:455:VAL:HG12	2.01	0.42
1:A:518:GLU:OE1	1:A:518:GLU:HA	2.19	0.42
1:A:177:CYS:O	1:A:180:PRO:HD2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LYS:HE3	1:A:382:GLU:OE2	2.20	0.42
1:A:216:VAL:CG2	3:A:4004:HLT:F2	2.57	0.42
1:A:95:GLU:O	1:A:96:PRO:C	2.56	0.42
1:A:480:SER:O	1:A:482:VAL:N	2.53	0.41
1:A:141:GLU:HA	1:A:144:ARG:HD3	2.03	0.41
1:A:37:GLU:H	1:A:37:GLU:CD	2.24	0.41
1:A:108:ASP:HB2	1:A:148:TYR:HE2	1.84	0.41
1:A:520:GLU:O	1:A:524:LYS:HG3	2.20	0.41
1:A:540:THR:HB	1:A:543:GLN:H	1.85	0.41
1:A:7:VAL:HG23	4:A:2004:HOH:O	2.19	0.41
1:A:282:PRO:O	1:A:283:LEU:C	2.59	0.41
1:A:373:VAL:HG12	1:A:374:PHE:HD1	1.85	0.41
1:A:356:THR:HG21	1:A:373:VAL:HG21	2.01	0.41
1:A:420:THR:HG23	1:A:530:VAL:HB	2.03	0.41
1:A:437:CYS:C	1:A:439:LYS:N	2.74	0.41
1:A:59:ALA:O	1:A:62:CYS:HB2	2.21	0.41
1:A:315:VAL:CG1	1:A:316:CYS:N	2.84	0.40
1:A:502:PHE:HE1	2:A:1005:MYR:H142	1.86	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	580/585 (99%)	527 (91%)	42 (7%)	11 (2%)	<b>8</b> <b>10</b>

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	PRO
1	A	367	HIS
1	A	479	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	364	ALA
1	A	278	CYS
1	A	481	LEU
1	A	564	LYS
1	A	499	PRO
1	A	502	PHE
1	A	95	GLU
1	A	469	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	467/511 (91%)	410 (88%)	57 (12%)	<b>5</b> <b>6</b>

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

Mol	Chain	Res	Type
1	A	5	SER
1	A	7	VAL
1	A	14	LEU
1	A	31	LEU
1	A	51	LYS
1	A	93	LYS
1	A	95	GLU
1	A	103	LEU
1	A	107	ASP
1	A	108	ASP
1	A	132	GLU
1	A	137	LYS
1	A	140	TYR
1	A	153	GLU
1	A	166	THR
1	A	179	LEU
1	A	185	LEU
1	A	193	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	203	LEU
1	A	225	LYS
1	A	232	SER
1	A	238	LEU
1	A	267	ASN
1	A	270	SER
1	A	282	PRO
1	A	287	SER
1	A	297	GLU
1	A	299	PRO
1	A	303	PRO
1	A	312	SER
1	A	314	ASP
1	A	334	TYR
1	A	337	ARG
1	A	351	LYS
1	A	373	VAL
1	A	378	LYS
1	A	408	LEU
1	A	414	LYS
1	A	415	VAL
1	A	426	VAL
1	A	436	LYS
1	A	453	LEU
1	A	455	VAL
1	A	457	LEU
1	A	459	GLN
1	A	467	THR
1	A	475	LYS
1	A	484	ARG
1	A	489	SER
1	A	498	VAL
1	A	509	PHE
1	A	512	ASP
1	A	514	CYS
1	A	520	GLU
1	A	538	LYS
1	A	544	LEU
1	A	566	THR

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

Mol	Chain	Res	Type
1	A	39	HIS
1	A	105	HIS
1	A	128	HIS
1	A	267	ASN
1	A	268	GLN
1	A	318	ASN
1	A	338	HIS
1	A	440	HIS
1	A	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
3	HLT	A	4006	-	4,6,6	1.50	1 (25%)	3,9,9	1.18	0
3	HLT	A	4007	-	4,6,6	1.49	1 (25%)	3,9,9	1.23	0
2	MYR	A	1002	-	9,12,15	0.25	0	8,12,15	0.94	1 (12%)
3	HLT	A	4008[A]	-	4,6,6	1.17	1 (25%)	3,9,9	1.21	0
2	MYR	A	1003	-	9,12,15	0.34	0	8,12,15	0.86	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HLT	A	4002	-	4,6,6	1.50	1 (25%)	3,9,9	1.24	0
2	MYR	A	1004	-	9,12,15	0.22	0	8,12,15	0.94	1 (12%)
3	HLT	A	4001	-	4,6,6	1.39	1 (25%)	3,9,9	1.27	0
2	MYR	A	1001	-	11,14,15	0.21	0	10,14,15	0.87	1 (10%)
3	HLT	A	4008[B]	-	4,6,6	0.76	0	3,9,9	1.12	0
3	HLT	A	4005	-	4,6,6	1.21	1 (25%)	3,9,9	1.28	0
3	HLT	A	4004	-	4,6,6	1.56	1 (25%)	3,9,9	1.28	0
2	MYR	A	1005	-	12,15,15	0.21	0	11,15,15	0.92	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HLT	A	4006	-	-	0/3/6/6	-
3	HLT	A	4007	-	-	3/3/6/6	-
2	MYR	A	1002	-	-	2/8/10/13	-
3	HLT	A	4008[A]	-	-	0/3/6/6	-
2	MYR	A	1003	-	-	5/8/10/13	-
3	HLT	A	4002	-	-	0/3/6/6	-
2	MYR	A	1004	-	-	5/8/10/13	-
3	HLT	A	4001	-	-	3/3/6/6	-
2	MYR	A	1001	-	-	7/10/12/13	-
3	HLT	A	4008[B]	-	-	0/3/6/6	-
3	HLT	A	4005	-	-	0/3/6/6	-
3	HLT	A	4004	-	-	0/3/6/6	-
2	MYR	A	1005	-	-	6/11/13/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4006	HLT	BR-C1	-2.97	1.86	1.96
3	A	4004	HLT	BR-C1	-2.89	1.87	1.96
3	A	4007	HLT	BR-C1	-2.76	1.87	1.96
3	A	4002	HLT	BR-C1	-2.74	1.87	1.96
3	A	4001	HLT	BR-C1	-2.69	1.87	1.96
3	A	4005	HLT	BR-C1	-2.40	1.88	1.96
3	A	4008[A]	HLT	BR-C1	-2.29	1.89	1.96



All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	MYR	C4-C3-C2	-2.48	104.13	113.76
2	A	1002	MYR	C4-C3-C2	-2.26	104.96	113.76
2	A	1001	MYR	C4-C3-C2	-2.24	105.06	113.76
2	A	1004	MYR	C4-C3-C2	-2.24	105.06	113.76
2	A	1003	MYR	C4-C3-C2	-2.09	105.64	113.76

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4007	HLT	CL-C1-C2-F1
3	A	4007	HLT	CL-C1-C2-F2
3	A	4007	HLT	CL-C1-C2-F3
2	A	1002	MYR	C1-C2-C3-C4
2	A	1003	MYR	C1-C2-C3-C4
2	A	1004	MYR	C1-C2-C3-C4
3	A	4001	HLT	CL-C1-C2-F1
3	A	4001	HLT	CL-C1-C2-F2
3	A	4001	HLT	CL-C1-C2-F3
2	A	1001	MYR	C1-C2-C3-C4
2	A	1005	MYR	C1-C2-C3-C4
2	A	1003	MYR	C5-C6-C7-C8
2	A	1001	MYR	C2-C3-C4-C5
2	A	1003	MYR	C6-C7-C8-C9
2	A	1001	MYR	C4-C5-C6-C7
2	A	1001	MYR	C5-C6-C7-C8
2	A	1004	MYR	C2-C3-C4-C5
2	A	1004	MYR	C6-C7-C8-C9
2	A	1001	MYR	C9-C10-C11-C12
2	A	1004	MYR	C4-C5-C6-C7
2	A	1001	MYR	C7-C8-C9-C10
2	A	1004	MYR	C11-C10-C9-C8
2	A	1005	MYR	C10-C11-C12-C13
2	A	1001	MYR	C10-C11-C12-C13
2	A	1005	MYR	C6-C7-C8-C9
2	A	1002	MYR	C2-C3-C4-C5
2	A	1005	MYR	C4-C5-C6-C7
2	A	1005	MYR	C9-C10-C11-C12
2	A	1003	MYR	C4-C5-C6-C7
2	A	1003	MYR	C11-C10-C9-C8
2	A	1005	MYR	C11-C10-C9-C8

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4006	HLT	2	0
3	A	4008[A]	HLT	1	0
3	A	4002	HLT	1	0
3	A	4001	HLT	2	0
2	A	1001	MYR	1	0
3	A	4008[B]	HLT	1	0
3	A	4005	HLT	1	0
3	A	4004	HLT	2	0
2	A	1005	MYR	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	582/585 (99%)	0.01	10 (1%) 70 68	23, 49, 82, 114	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ASP	3.5
1	A	568	PHE	3.2
1	A	364	ALA	2.8
1	A	302	LEU	2.6
1	A	575	LEU	2.6
1	A	561	ALA	2.5
1	A	555	VAL	2.5
1	A	299	PRO	2.4
1	A	513	ILE	2.1
1	A	553	ALA	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MYR	A	1002	13/16	0.82	0.26	52,54,69,70	0
3	HLT	A	4002	7/7	0.86	0.20	62,62,66,71	7
3	HLT	A	4001	7/7	0.86	0.27	55,59,61,64	7
2	MYR	A	1003	13/16	0.87	0.21	40,44,53,54	0
3	HLT	A	4008[A]	7/7	0.88	0.21	55,56,61,65	7
2	MYR	A	1004	13/16	0.88	0.21	52,54,65,66	0
3	HLT	A	4006	7/7	0.88	0.18	62,62,64,69	7
3	HLT	A	4008[B]	7/7	0.88	0.21	50,52,57,64	7
3	HLT	A	4004	7/7	0.88	0.25	63,63,64,70	7
3	HLT	A	4005	7/7	0.90	0.25	57,60,62,65	7
2	MYR	A	1005	16/16	0.90	0.27	55,59,62,62	0
3	HLT	A	4007	7/7	0.91	0.24	43,46,47,60	7
2	MYR	A	1001	15/16	0.91	0.22	46,53,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.