



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3B9M
Title : Human serum albumin complexed with myristate, 3'-azido-3'-deoxythymidine (AZT) and salicylic acid
Authors : Zhu, L.; Yang, F.; Chen, L.; Meehan, E.J.; Huang, M.
Deposited on : 2007-11-05
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

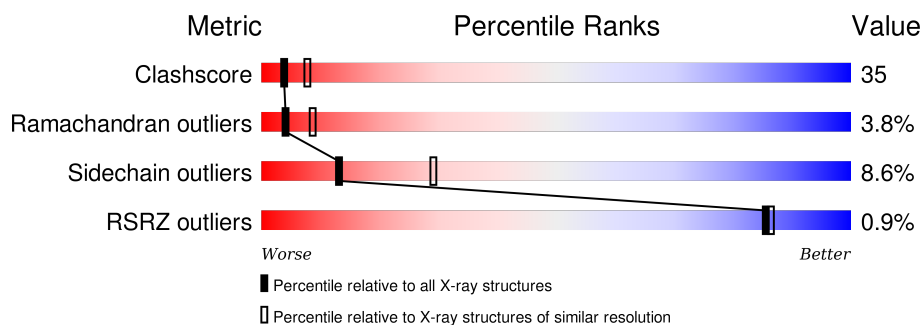
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 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 $\leq 5\%$. 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
2	MYR	A	1001	-	-	-	X
2	MYR	A	1002	-	-	-	X
2	MYR	A	1003	-	-	X	X
2	MYR	A	1004	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYR	A	1005	-	-	-	X
2	MYR	A	1006	-	-	-	X
3	AZZ	A	1009	-	-	-	X
4	SAL	A	1100	-	-	-	X
4	SAL	A	1200	-	-	-	X

2 Entry composition [i](#)

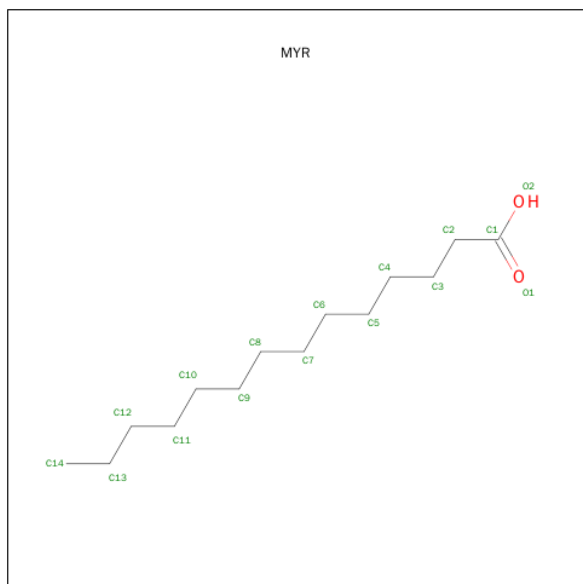
There are 4 unique types of molecules in this entry. The entry contains 4765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4630	2923	783	883	41			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



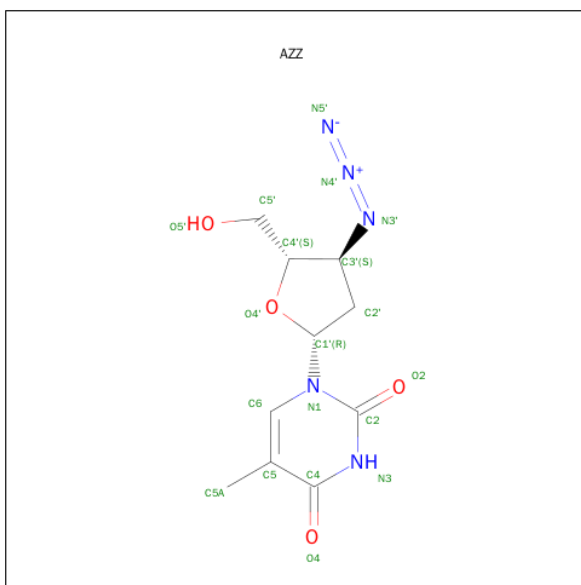
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		

Continued on next page...

Continued from previous page...

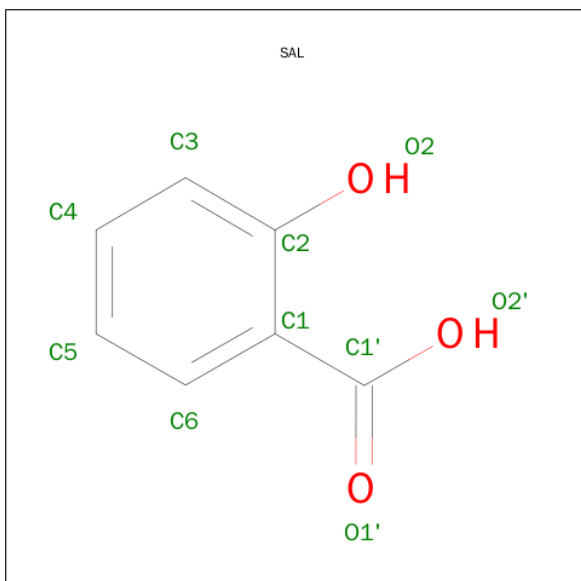
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is 3'-AZIDO-3'-DEOXYTHYMIDINE (three-letter code: AZZ) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	7	3		
4	A	1	Total	C	O	0	0
			10	7	3		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.54Å 38.46Å 95.37Å 90.00° 104.92° 90.00°	Depositor
Resolution (Å)	46.08 – 2.70 46.08 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.9 (46.08-2.70) 88.0 (46.08-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.316 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 15854 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4765	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: AZZ, MYR, SAL

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	0.41	0/4720	0.66	0/6366

There are no bond length outliers.

There are no bond angle outliers.

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	4630	0	4552	321	0
2	A	96	0	162	53	0
3	A	19	0	13	2	0
4	A	20	0	9	1	0
All	All	4765	0	4736	331	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 35.

All (331) 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:403:PHE:CE2	2:A:1003:MYR:H141	1.66	1.29
2:A:1004:MYR:C14	2:A:1004:MYR:H92	1.69	1.22
2:A:1004:MYR:C14	2:A:1004:MYR:C9	2.30	1.10
1:A:403:PHE:HE2	2:A:1003:MYR:H141	0.91	1.07
2:A:1004:MYR:H143	2:A:1004:MYR:H92	1.24	1.05
2:A:1004:MYR:H143	2:A:1004:MYR:C9	1.91	1.00
2:A:1004:MYR:C9	2:A:1004:MYR:H142	1.91	1.00
1:A:403:PHE:HE2	2:A:1003:MYR:C14	1.79	0.94
1:A:118:PRO:HG2	1:A:123:MET:HG3	1.50	0.94
1:A:424:VAL:O	1:A:428:ARG:HG3	1.69	0.93
1:A:564:LYS:HD3	1:A:564:LYS:H	1.37	0.88
1:A:150:TYR:H	1:A:196:GLN:HE22	1.20	0.87
1:A:411:TYR:OH	2:A:1004:MYR:O1	1.93	0.86
1:A:432:LYS:O	1:A:435:SER:N	2.07	0.86
1:A:388:ILE:CD1	2:A:1003:MYR:H81	2.07	0.85
2:A:1006:MYR:H61	2:A:1006:MYR:H22	1.59	0.84
2:A:1004:MYR:H91	2:A:1004:MYR:H142	1.60	0.82
1:A:411:TYR:CE1	2:A:1004:MYR:H82	2.16	0.80
1:A:299:PRO:HB2	1:A:302:LEU:HG	1.63	0.79
1:A:388:ILE:HD13	2:A:1003:MYR:H81	1.64	0.79
1:A:403:PHE:CE2	2:A:1003:MYR:C14	2.58	0.78
1:A:546:ALA:O	1:A:548:MET:N	2.16	0.77
1:A:49:PHE:O	1:A:52:THR:HB	1.84	0.77
1:A:342:SER:HB3	1:A:446:MET:HG2	1.66	0.77
1:A:138:TYR:O	1:A:142:ILE:HG12	1.84	0.77
1:A:557:LYS:HA	1:A:557:LYS:HE3	1.67	0.76
1:A:141:GLU:OE1	1:A:144:ARG:HD3	1.86	0.76
1:A:398:LEU:HB3	1:A:402:LYS:HB3	1.65	0.76
1:A:299:PRO:HD2	1:A:302:LEU:HD11	1.68	0.76
1:A:175:ALA:HB1	1:A:179:LEU:HD22	1.68	0.76
1:A:348:ARG:HH22	2:A:1003:MYR:C1	2.01	0.74
1:A:10:ARG:HB3	1:A:10:ARG:HH11	1.53	0.72
1:A:344:VAL:HG22	2:A:1003:MYR:O2	1.89	0.72
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.71	0.72
1:A:520:GLU:O	1:A:524:LYS:HG3	1.91	0.71
1:A:42:LEU:HD22	1:A:73:LYS:HD2	1.71	0.70
1:A:510:HIS:O	1:A:513:ILE:HG23	1.90	0.70
1:A:485:ARG:HE	2:A:1003:MYR:H31	1.57	0.70
1:A:485:ARG:NE	2:A:1003:MYR:H31	2.07	0.69
1:A:10:ARG:HD2	1:A:66:LEU:CD1	2.22	0.69
1:A:95:GLU:OE1	1:A:98:ARG:NH2	2.26	0.69
1:A:564:LYS:CD	1:A:564:LYS:H	2.05	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PRO:O	1:A:300:ALA:HB3	1.93	0.69
1:A:576:VAL:O	1:A:580:GLN:HG2	1.93	0.68
1:A:10:ARG:HD2	1:A:66:LEU:HD12	1.74	0.68
1:A:420:THR:HB	1:A:421:PRO:HD3	1.74	0.68
1:A:276:LYS:HD3	1:A:277:GLU:N	2.08	0.68
1:A:564:LYS:HD3	1:A:564:LYS:N	2.09	0.67
1:A:209:ARG:HH12	2:A:1006:MYR:H21	1.58	0.67
1:A:212:LYS:O	1:A:216:VAL:HG23	1.95	0.67
1:A:10:ARG:O	1:A:14:LEU:HB2	1.93	0.67
1:A:536:LYS:HG2	1:A:583:LEU:HB3	1.78	0.66
1:A:120:VAL:HG21	1:A:175:ALA:HB2	1.77	0.66
1:A:217:ALA:O	1:A:221:GLN:HB2	1.96	0.66
1:A:214:TRP:CH2	1:A:218:ARG:HD3	2.30	0.66
2:A:1006:MYR:H22	2:A:1006:MYR:C6	2.25	0.66
1:A:237:ASP:HB3	1:A:260:LEU:HD13	1.77	0.66
1:A:152:PRO:O	1:A:156:PHE:HD1	1.79	0.66
1:A:519:LYS:O	1:A:523:ILE:HG12	1.96	0.66
1:A:4:LYS:HD2	1:A:57:GLU:OE1	1.96	0.66
1:A:545:LYS:HA	1:A:548:MET:CE	2.26	0.65
1:A:517:SER:OG	1:A:520:GLU:HG2	1.97	0.65
1:A:551:PHE:HA	1:A:554:PHE:HB3	1.79	0.65
1:A:6:GLU:O	1:A:10:ARG:HG3	1.97	0.65
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.31	0.65
1:A:31:LEU:HD22	1:A:31:LEU:H	1.59	0.64
1:A:276:LYS:HD3	1:A:276:LYS:C	2.17	0.64
1:A:536:LYS:HG2	1:A:583:LEU:CB	2.28	0.64
1:A:439:LYS:HE3	1:A:439:LYS:HA	1.79	0.64
1:A:348:ARG:NH1	2:A:1003:MYR:O1	2.31	0.63
1:A:290:ILE:O	1:A:293:VAL:HG12	1.99	0.63
1:A:567:CYS:O	1:A:571:GLU:HB2	1.98	0.63
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.80	0.63
1:A:426:VAL:HG11	2:A:1004:MYR:H112	1.80	0.63
1:A:31:LEU:HD21	1:A:74:LEU:CD1	2.29	0.62
1:A:119:GLU:HB2	1:A:122:VAL:CG1	2.29	0.62
1:A:432:LYS:O	1:A:434:GLY:N	2.32	0.62
1:A:516:LEU:HD22	1:A:520:GLU:CB	2.30	0.62
1:A:253:CYS:O	1:A:257:ARG:HG3	2.00	0.62
1:A:558:CYS:HB3	1:A:568:PHE:CE2	2.34	0.61
1:A:137:LYS:O	1:A:140:TYR:HB3	2.00	0.61
1:A:209:ARG:NH1	2:A:1006:MYR:H21	2.15	0.61
1:A:119:GLU:HB2	1:A:122:VAL:HG13	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:HD1	2:A:1002:MYR:H142	1.64	0.61
1:A:540:THR:C	1:A:542:GLU:H	2.04	0.61
1:A:199:LYS:HD3	1:A:242:HIS:CE1	2.36	0.61
1:A:426:VAL:O	1:A:430:LEU:HB2	2.00	0.61
1:A:25:ILE:O	1:A:29:GLN:HG3	2.01	0.60
1:A:160:ARG:HH22	1:A:188:GLU:CD	2.04	0.60
1:A:344:VAL:HG12	1:A:450:GLU:OE2	2.01	0.60
1:A:161:TYR:CD2	2:A:1001:MYR:H111	2.36	0.60
1:A:436:LYS:HD3	1:A:452:TYR:CZ	2.36	0.60
1:A:389:LYS:O	1:A:393:GLU:HG3	2.02	0.60
1:A:540:THR:C	1:A:542:GLU:N	2.53	0.60
1:A:348:ARG:HH12	2:A:1003:MYR:C1	2.15	0.60
1:A:36:PHE:CE1	1:A:137:LYS:HA	2.36	0.60
1:A:107:ASP:O	1:A:147:PRO:HG3	2.02	0.60
1:A:311:GLU:O	1:A:312:SER:O	2.20	0.59
1:A:513:ILE:C	1:A:513:ILE:HD12	2.22	0.59
1:A:410:ARG:O	1:A:414:LYS:HG2	2.01	0.59
1:A:152:PRO:O	1:A:155:LEU:HB3	2.01	0.59
1:A:178:LEU:HD11	1:A:182:LEU:HD21	1.85	0.59
1:A:433:VAL:HG11	1:A:453:LEU:HD13	1.83	0.59
1:A:381:VAL:O	1:A:385:GLN:HG3	2.03	0.59
1:A:315:VAL:HG12	1:A:316:CYS:N	2.18	0.58
1:A:349:LEU:O	1:A:352:THR:HB	2.02	0.58
1:A:378:LYS:O	1:A:382:GLU:HG3	2.03	0.58
1:A:545:LYS:HA	1:A:548:MET:HE3	1.84	0.58
1:A:250:LEU:O	1:A:250:LEU:HD12	2.03	0.58
1:A:541:LYS:O	1:A:545:LYS:HB2	2.04	0.58
1:A:135:LEU:N	1:A:135:LEU:HD22	2.18	0.57
1:A:225:LYS:HE3	1:A:297:GLU:O	2.04	0.57
1:A:352:THR:HG22	1:A:353:TYR:N	2.19	0.57
1:A:329:MET:O	1:A:333:GLU:HG2	2.03	0.57
1:A:184:GLU:O	1:A:188:GLU:HB2	2.05	0.56
1:A:335:ALA:HB2	1:A:346:LEU:HD13	1.87	0.56
1:A:16:GLU:OE1	1:A:51:LYS:HE2	2.06	0.56
1:A:81:ARG:NH2	1:A:89:ASP:OD1	2.38	0.56
1:A:299:PRO:HB2	1:A:302:LEU:CG	2.33	0.56
1:A:521:ARG:O	1:A:525:LYS:HG3	2.06	0.56
1:A:215:ALA:O	1:A:219:LEU:HB2	2.06	0.56
1:A:569:ALA:O	1:A:573:LYS:HG2	2.05	0.56
1:A:436:LYS:HD3	1:A:452:TYR:OH	2.06	0.56
1:A:462:VAL:O	1:A:466:LYS:HD3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:SER:HG	1:A:520:GLU:HG2	1.70	0.55
1:A:120:VAL:HG21	1:A:175:ALA:CB	2.36	0.55
1:A:64:LYS:HE2	1:A:68:THR:HG21	1.87	0.55
1:A:155:LEU:HD23	1:A:284:LEU:HD21	1.88	0.55
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.89	0.55
1:A:299:PRO:O	1:A:300:ALA:CB	2.55	0.55
1:A:303:PRO:O	1:A:337:ARG:NH1	2.40	0.55
1:A:409:VAL:O	1:A:413:LYS:HG3	2.07	0.55
1:A:244:GLU:HB3	1:A:252:GLU:OE2	2.08	0.54
1:A:161:TYR:CG	2:A:1001:MYR:H111	2.42	0.54
1:A:536:LYS:HB2	1:A:536:LYS:NZ	2.22	0.54
1:A:31:LEU:HD21	1:A:74:LEU:HD12	1.87	0.54
1:A:364:ALA:O	1:A:366:PRO:HD3	2.07	0.54
1:A:107:ASP:OD2	1:A:110:PRO:HA	2.08	0.54
1:A:405:ASN:HD22	1:A:529:LEU:HD22	1.72	0.54
1:A:403:PHE:CZ	2:A:1003:MYR:H141	2.36	0.53
1:A:513:ILE:O	1:A:513:ILE:HD12	2.08	0.53
1:A:536:LYS:HZ2	1:A:536:LYS:HB2	1.72	0.53
1:A:509:PHE:O	1:A:568:PHE:HB3	2.09	0.53
1:A:522:GLN:O	1:A:526:GLN:HG3	2.09	0.53
1:A:504:ALA:O	1:A:508:THR:HG23	2.08	0.53
1:A:503:ASN:OD1	1:A:505:GLU:HB3	2.09	0.53
1:A:564:LYS:O	1:A:566:THR:N	2.41	0.53
1:A:580:GLN:HE21	1:A:580:GLN:HA	1.74	0.52
1:A:445:ARG:O	1:A:448:CYS:HB3	2.09	0.52
1:A:467:THR:O	1:A:469:VAL:HG23	2.09	0.52
1:A:315:VAL:CG1	1:A:316:CYS:N	2.71	0.52
1:A:199:LYS:HD3	1:A:242:HIS:HE1	1.75	0.52
1:A:436:LYS:HD3	1:A:452:TYR:CE2	2.45	0.52
1:A:142:ILE:HG13	2:A:1001:MYR:H132	1.92	0.52
1:A:401:TYR:OH	1:A:525:LYS:HD2	2.09	0.52
1:A:540:THR:O	1:A:544:LEU:HB2	2.10	0.51
1:A:551:PHE:O	1:A:555:VAL:HG23	2.10	0.51
1:A:277:GLU:OE2	1:A:277:GLU:HA	2.10	0.51
1:A:348:ARG:NH2	2:A:1003:MYR:O2	2.39	0.51
1:A:199:LYS:HD2	3:A:1009:AZZ:H5A	1.91	0.51
1:A:68:THR:OG1	1:A:95:GLU:HG2	2.10	0.51
1:A:449:ALA:O	1:A:453:LEU:HB2	2.11	0.51
1:A:303:PRO:C	1:A:337:ARG:HH12	2.13	0.51
1:A:373:VAL:CG1	1:A:374:PHE:HD1	2.24	0.51
1:A:344:VAL:HG13	2:A:1003:MYR:O2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:THR:HB	1:A:542:GLU:HB2	1.93	0.51
1:A:455:VAL:HG23	1:A:456:VAL:N	2.26	0.51
1:A:444:LYS:O	1:A:447:PRO:HD2	2.11	0.51
1:A:502:PHE:CG	1:A:503:ASN:N	2.80	0.50
1:A:139:LEU:HD12	2:A:1001:MYR:H142	1.93	0.50
1:A:564:LYS:HG2	1:A:565:GLU:N	2.26	0.50
1:A:118:PRO:HG2	1:A:123:MET:CG	2.33	0.50
1:A:178:LEU:O	1:A:181:LYS:HB2	2.12	0.50
1:A:344:VAL:CG2	2:A:1003:MYR:O2	2.59	0.50
1:A:545:LYS:C	1:A:545:LYS:HE2	2.32	0.50
1:A:177:CYS:O	1:A:181:LYS:HD2	2.12	0.50
1:A:378:LYS:N	1:A:379:PRO:HD2	2.27	0.50
1:A:174:LYS:O	1:A:177:CYS:N	2.32	0.49
1:A:31:LEU:HD21	1:A:74:LEU:HD11	1.94	0.49
1:A:445:ARG:O	1:A:448:CYS:N	2.45	0.49
1:A:10:ARG:HD2	1:A:66:LEU:HD11	1.94	0.49
1:A:41:LYS:O	1:A:45:GLU:HG3	2.13	0.49
1:A:31:LEU:HB2	1:A:39:HIS:HE1	1.77	0.49
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.65	0.49
1:A:419:SER:OG	1:A:421:PRO:HD2	2.13	0.49
1:A:373:VAL:CG1	1:A:374:PHE:N	2.76	0.49
1:A:434:GLY:O	1:A:438:CYS:HB2	2.12	0.49
1:A:150:TYR:OH	2:A:1002:MYR:H21	2.13	0.49
1:A:131:GLU:O	1:A:135:LEU:CD2	2.61	0.49
1:A:293:VAL:HG22	1:A:294:GLU:N	2.27	0.48
1:A:394:LEU:HD23	1:A:403:PHE:HD1	1.77	0.48
1:A:257:ARG:HH21	1:A:287:SER:HB3	1.77	0.48
1:A:313:LYS:O	1:A:314:ASP:HB2	2.13	0.48
1:A:545:LYS:C	1:A:546:ALA:O	2.51	0.48
1:A:404:GLN:HG2	1:A:431:GLY:HA3	1.96	0.48
1:A:485:ARG:CZ	2:A:1003:MYR:H31	2.44	0.48
1:A:513:ILE:HG13	1:A:514:CYS:N	2.29	0.48
1:A:71:GLY:HA3	1:A:98:ARG:NH2	2.29	0.48
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.79	0.48
1:A:348:ARG:CZ	2:A:1003:MYR:O1	2.62	0.47
1:A:507:PHE:O	1:A:509:PHE:CE1	2.66	0.47
1:A:554:PHE:HE2	1:A:572:GLY:HA2	1.79	0.47
1:A:332:TYR:OH	1:A:336:ARG:NH2	2.47	0.47
1:A:580:GLN:NE2	1:A:580:GLN:HA	2.29	0.47
1:A:452:TYR:O	1:A:455:VAL:HG22	2.15	0.47
4:A:1200:SAL:O2	4:A:1200:SAL:O1'	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:NH2	2:A:1003:MYR:C1	2.74	0.47
1:A:254:ALA:HB1	2:A:1002:MYR:H41	1.97	0.47
1:A:408:LEU:CD2	1:A:526:GLN:HB3	2.43	0.47
1:A:38:ASP:O	1:A:41:LYS:CB	2.63	0.47
1:A:353:TYR:CZ	1:A:357:LEU:HD11	2.49	0.47
1:A:335:ALA:CB	1:A:346:LEU:HD13	2.44	0.47
1:A:198:LEU:HD12	1:A:198:LEU:O	2.15	0.47
1:A:31:LEU:HD22	1:A:31:LEU:N	2.29	0.47
1:A:580:GLN:HE21	1:A:580:GLN:CA	2.28	0.47
1:A:257:ARG:HH21	1:A:287:SER:CB	2.28	0.47
1:A:393:GLU:O	1:A:397:GLN:HG3	2.16	0.46
1:A:73:LYS:O	1:A:76:THR:HB	2.15	0.46
1:A:511:ALA:HA	1:A:568:PHE:CE2	2.50	0.46
1:A:468:PRO:O	1:A:469:VAL:HG23	2.15	0.46
1:A:90:CYS:O	1:A:98:ARG:HG3	2.15	0.46
1:A:114:ARG:CZ	1:A:116:VAL:HG12	2.46	0.46
1:A:348:ARG:HG2	1:A:380:LEU:HD21	1.97	0.46
1:A:68:THR:HA	1:A:95:GLU:OE1	2.15	0.46
1:A:237:ASP:O	1:A:241:VAL:HG23	2.15	0.46
1:A:37:GLU:CD	1:A:37:GLU:H	2.19	0.46
1:A:536:LYS:HG2	1:A:583:LEU:HB2	1.98	0.46
1:A:366:PRO:O	1:A:369:CYS:N	2.49	0.46
1:A:139:LEU:HD13	1:A:158:ALA:HB2	1.98	0.46
1:A:244:GLU:O	1:A:247:HIS:HB3	2.16	0.46
1:A:370:TYR:HD1	1:A:370:TYR:O	1.99	0.46
1:A:150:TYR:HB2	3:A:1009:AZZ:H2'	1.97	0.46
1:A:281:LYS:HB3	1:A:282:PRO:HD2	1.97	0.46
2:A:1004:MYR:H111	2:A:1004:MYR:H143	1.24	0.46
1:A:38:ASP:O	1:A:41:LYS:HB3	2.16	0.46
1:A:473:VAL:HG12	1:A:473:VAL:O	2.16	0.46
1:A:185:LEU:HA	1:A:185:LEU:HD12	1.73	0.46
1:A:558:CYS:HB3	1:A:568:PHE:CD2	2.52	0.45
1:A:485:ARG:NH2	2:A:1003:MYR:H31	2.31	0.45
1:A:567:CYS:C	1:A:569:ALA:H	2.20	0.45
1:A:432:LYS:O	1:A:433:VAL:C	2.54	0.45
1:A:392:CYS:O	1:A:396:GLU:HG3	2.16	0.45
1:A:360:CYS:SG	1:A:370:TYR:HB3	2.57	0.45
1:A:460:LEU:HD21	2:A:1004:MYR:H122	1.99	0.45
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.88	0.45
1:A:296:ASP:OD1	1:A:297:GLU:N	2.49	0.44
1:A:378:LYS:HA	1:A:378:LYS:HD3	1.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:VAL:O	1:A:329:MET:HG3	2.17	0.44
1:A:469:VAL:O	1:A:469:VAL:HG12	2.17	0.44
1:A:345:LEU:HA	1:A:348:ARG:NH1	2.32	0.44
1:A:123:MET:CE	2:A:1001:MYR:H62	2.48	0.44
1:A:304:SER:CA	1:A:337:ARG:HH12	2.30	0.44
1:A:557:LYS:CA	1:A:557:LYS:HE3	2.43	0.44
1:A:250:LEU:C	1:A:250:LEU:HD12	2.37	0.44
1:A:14:LEU:HD21	2:A:1002:MYR:H71	1.99	0.44
1:A:131:GLU:O	1:A:135:LEU:HD23	2.17	0.44
1:A:35:PRO:O	1:A:38:ASP:HB2	2.18	0.44
1:A:187:ASP:OD1	1:A:432:LYS:NZ	2.42	0.44
1:A:186:ARG:O	1:A:187:ASP:C	2.55	0.44
1:A:434:GLY:H	2:A:1003:MYR:H142	1.82	0.44
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.53	0.44
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.58	0.44
1:A:461:CYS:O	1:A:465:GLU:N	2.50	0.44
1:A:259:ASP:O	1:A:262:LYS:HB2	2.17	0.44
1:A:403:PHE:CZ	2:A:1003:MYR:C13	3.00	0.44
1:A:81:ARG:HG3	1:A:81:ARG:O	2.18	0.44
1:A:464:HIS:HE1	1:A:474:THR:OG1	2.01	0.44
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.77	0.43
1:A:479:GLU:HG2	1:A:480:SER:H	1.83	0.43
1:A:334:TYR:CZ	1:A:349:LEU:HD13	2.53	0.43
1:A:403:PHE:HZ	2:A:1003:MYR:C13	2.32	0.43
1:A:412:THR:HG21	1:A:533:VAL:HB	2.00	0.43
1:A:307:ALA:O	1:A:312:SER:HB3	2.19	0.43
1:A:179:LEU:C	1:A:181:LYS:H	2.22	0.43
1:A:516:LEU:HD22	1:A:520:GLU:HB3	2.01	0.43
1:A:479:GLU:OE1	1:A:483:ASN:HB3	2.18	0.43
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.54	0.43
1:A:394:LEU:HD22	1:A:403:PHE:CE1	2.54	0.43
1:A:299:PRO:HG2	1:A:302:LEU:HD21	1.99	0.43
1:A:298:MET:HB2	1:A:299:PRO:HD2	2.01	0.43
1:A:366:PRO:O	1:A:367:HIS:C	2.57	0.43
1:A:123:MET:HE2	1:A:165:PHE:CE1	2.54	0.43
1:A:150:TYR:H	1:A:196:GLN:NE2	2.02	0.43
1:A:174:LYS:O	1:A:177:CYS:HB3	2.18	0.42
1:A:394:LEU:HD23	1:A:398:LEU:HD12	2.01	0.42
1:A:515:THR:O	1:A:515:THR:HG23	2.19	0.42
1:A:388:ILE:O	1:A:389:LYS:C	2.55	0.42
1:A:313:LYS:HG2	1:A:314:ASP:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HG22	1:A:82:GLU:CD	2.40	0.42
1:A:341:TYR:HD2	1:A:346:LEU:HD21	1.85	0.42
1:A:206:PHE:CG	1:A:481:LEU:HD11	2.55	0.42
1:A:462:VAL:O	1:A:465:GLU:HB3	2.19	0.42
1:A:100:GLU:OE2	1:A:247:HIS:CE1	2.73	0.42
1:A:160:ARG:NH2	1:A:188:GLU:OE1	2.49	0.42
1:A:345:LEU:HD12	1:A:345:LEU:O	2.19	0.42
1:A:60:GLU:O	1:A:61:ASN:HB2	2.20	0.42
1:A:395:PHE:C	1:A:395:PHE:CD1	2.93	0.42
1:A:540:THR:HB	1:A:543:GLN:H	1.85	0.42
1:A:413:LYS:HG2	1:A:533:VAL:CG1	2.50	0.42
1:A:348:ARG:NH2	2:A:1003:MYR:O1	2.52	0.41
1:A:22:LEU:HD13	2:A:1002:MYR:H82	2.02	0.41
1:A:238:LEU:O	1:A:241:VAL:HB	2.21	0.41
1:A:97:GLU:CD	1:A:97:GLU:N	2.73	0.41
1:A:388:ILE:HD11	2:A:1003:MYR:H81	1.98	0.41
1:A:429:ASN:O	1:A:433:VAL:HG23	2.20	0.41
1:A:141:GLU:HA	1:A:144:ARG:HD3	2.03	0.41
1:A:535:HIS:CD2	1:A:536:LYS:NZ	2.88	0.41
1:A:408:LEU:HD11	1:A:530:VAL:CG2	2.50	0.41
1:A:469:VAL:O	1:A:469:VAL:CG1	2.69	0.41
1:A:473:VAL:O	1:A:477:CYS:HB2	2.21	0.41
1:A:206:PHE:CZ	1:A:481:LEU:HG	2.55	0.41
1:A:304:SER:O	1:A:306:ALA:N	2.54	0.41
1:A:302:LEU:HA	1:A:303:PRO:HD3	1.82	0.41
1:A:304:SER:HA	1:A:337:ARG:HH12	1.85	0.41
1:A:557:LYS:HG3	1:A:557:LYS:O	2.20	0.41
1:A:97:GLU:O	1:A:98:ARG:C	2.59	0.41
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.41
1:A:307:ALA:O	1:A:312:SER:CB	2.68	0.41
1:A:541:LYS:HA	1:A:541:LYS:HD2	1.98	0.41
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.56	0.41
1:A:251:LEU:HD21	2:A:1002:MYR:H101	2.03	0.40
1:A:6:GLU:O	1:A:10:ARG:CG	2.67	0.40
1:A:153:GLU:O	1:A:157:PHE:HD2	2.04	0.40
1:A:6:GLU:OE1	1:A:66:LEU:HB2	2.21	0.40
1:A:535:HIS:CD2	1:A:536:LYS:HZ2	2.40	0.40
1:A:549:ASP:C	1:A:551:PHE:N	2.75	0.40
1:A:402:LYS:HE2	1:A:402:LYS:HB2	1.92	0.40
1:A:123:MET:HE1	2:A:1001:MYR:H62	2.03	0.40
1:A:452:TYR:O	1:A:456:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TYR:CD1	2:A:1004:MYR:H82	2.56	0.40
1:A:411:TYR:CE2	1:A:430:LEU:HD23	2.57	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%)	495 (85%)	63 (11%)	22 (4%)	4 9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	LEU
1	A	303	PRO
1	A	311	GLU
1	A	312	SER
1	A	433	VAL
1	A	445	ARG
1	A	564	LYS
1	A	85	GLY
1	A	283	LEU
1	A	286	LYS
1	A	300	ALA
1	A	305	LEU
1	A	565	GLU
1	A	484	ARG
1	A	174	LYS
1	A	277	GLU
1	A	469	VAL
1	A	479	GLU
1	A	546	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	547	VAL
1	A	389	LYS
1	A	442	GLU

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	509/511 (100%)	465 (91%)	44 (9%)	13	29

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

Mol	Chain	Res	Type
1	A	3	HIS
1	A	10	ARG
1	A	14	LEU
1	A	31	LEU
1	A	38	ASP
1	A	57	GLU
1	A	79	THR
1	A	103	LEU
1	A	108	ASP
1	A	122	VAL
1	A	123	MET
1	A	132	GLU
1	A	153	GLU
1	A	170	GLN
1	A	179	LEU
1	A	208	GLU
1	A	238	LEU
1	A	250	LEU
1	A	257	ARG
1	A	276	LYS
1	A	315	VAL
1	A	336	ARG
1	A	368	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	373	VAL
1	A	378	LYS
1	A	394	LEU
1	A	398	LEU
1	A	402	LYS
1	A	439	LYS
1	A	442	GLU
1	A	453	LEU
1	A	457	LEU
1	A	467	THR
1	A	481	LEU
1	A	501	GLU
1	A	509	PHE
1	A	513	ILE
1	A	536	LYS
1	A	545	LYS
1	A	549	ASP
1	A	554	PHE
1	A	557	LYS
1	A	564	LYS
1	A	570	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	39	HIS
1	A	105	HIS
1	A	170	GLN
1	A	196	GLN
1	A	242	HIS
1	A	247	HIS
1	A	338	HIS
1	A	367	HIS
1	A	429	ASN
1	A	580	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	MYR	A	1001	-	12,15,15	0.23	0	12,15,15	0.97	1 (8%)
2	MYR	A	1002	-	12,15,15	0.25	0	12,15,15	1.24	1 (8%)
2	MYR	A	1003	-	12,15,15	0.23	0	12,15,15	0.64	0
2	MYR	A	1004	-	12,15,15	0.37	0	12,15,15	1.43	3 (25%)
2	MYR	A	1005	-	12,15,15	0.12	0	12,15,15	1.04	0
2	MYR	A	1006	-	12,15,15	0.22	0	12,15,15	0.87	0
3	AZZ	A	1009	-	14,20,20	1.73	3 (21%)	16,28,28	2.38	2 (12%)
4	SAL	A	1100	-	7,10,10	2.97	6 (85%)	10,13,13	1.35	1 (10%)
4	SAL	A	1200	-	7,10,10	2.58	5 (71%)	10,13,13	2.00	3 (30%)

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	MYR	A	1001	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1002	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1003	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1004	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1005	-	-	0/11/13/13	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	1006	-	-	0/11/13/13	0/0/0/0
3	AZZ	A	1009	-	-	1/5/21/21	0/2/2/2
4	SAL	A	1100	-	-	0/0/4/4	0/1/1/1
4	SAL	A	1200	-	-	0/0/4/4	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1200	SAL	C3-C2	-3.97	1.32	1.39
3	A	1009	AZZ	N4'-N3'	-3.55	1.13	1.23
4	A	1200	SAL	O2-C2	-3.21	1.29	1.36
4	A	1200	SAL	C6-C1	-2.89	1.35	1.39
4	A	1200	SAL	C1-C2	-2.36	1.33	1.40
4	A	1200	SAL	C5-C6	-2.21	1.34	1.38
4	A	1100	SAL	C1-C2	2.26	1.47	1.40
4	A	1100	SAL	C4-C3	2.28	1.43	1.38
3	A	1009	AZZ	C4-N3	2.31	1.37	1.33
4	A	1100	SAL	C5-C4	2.79	1.45	1.38
4	A	1100	SAL	C5-C6	3.63	1.46	1.38
4	A	1100	SAL	C3-C2	3.82	1.46	1.39
4	A	1100	SAL	C6-C1	3.95	1.46	1.39
3	A	1009	AZZ	C6-N1	4.30	1.41	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1009	AZZ	C5-C4-N3	-4.99	119.58	125.14
4	A	1200	SAL	C4-C3-C2	-3.71	115.28	120.04
4	A	1200	SAL	C2-C1-C1'	-3.53	117.98	121.60
2	A	1002	MYR	C4-C3-C2	-2.58	102.99	113.90
2	A	1004	MYR	C10-C9-C8	-2.29	102.72	114.53
2	A	1004	MYR	C8-C7-C6	-2.24	102.99	114.53
2	A	1004	MYR	C14-C13-C12	-2.22	96.02	113.44
2	A	1001	MYR	C9-C8-C7	-2.17	103.31	114.53
4	A	1100	SAL	C2-C1-C1'	2.35	124.01	121.60
4	A	1200	SAL	C5-C4-C3	2.44	123.75	120.19
3	A	1009	AZZ	C4-N3-C2	7.04	121.33	115.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1009	AZZ	C3'-N3'-N4'-N5'

There are no ring outliers.

7 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	MYR	6	0
2	A	1002	MYR	6	0
2	A	1003	MYR	25	0
2	A	1004	MYR	12	0
2	A	1006	MYR	4	0
3	A	1009	AZZ	2	0
4	A	1200	SAL	1	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, 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	582/585 (99%)	-0.08	5 (0%) 85 86	28, 62, 108, 144	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	LEU	2.9
1	A	138	TYR	2.5
1	A	580	GLN	2.5
1	A	557	LYS	2.3
1	A	570	GLU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	AZZ	A	1009	19/19	0.68	0.58	11.12	107,114,120,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SAL	A	1100	10/10	0.78	0.42	10.90	80,91,97,97	0
2	MYR	A	1003	16/16	0.71	0.50	10.46	52,59,64,64	0
2	MYR	A	1006	16/16	0.76	0.48	9.59	65,76,106,106	0
2	MYR	A	1004	16/16	0.77	0.47	7.35	53,58,67,68	0
2	MYR	A	1002	16/16	0.83	0.44	5.50	58,66,86,87	0
2	MYR	A	1005	16/16	0.78	0.47	4.13	56,61,74,74	0
2	MYR	A	1001	16/16	0.82	0.33	3.03	64,69,73,73	0
4	SAL	A	1200	10/10	0.85	0.27	2.88	58,67,92,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.