Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 03:06 AM EDT

PDB ID	:	1AQL
Title	:	CRYSTAL STRUCTURE OF BOVINE BILE-SALT ACTIVATED LIPASE COMPLEXED WITH TAUROCHOLATE
Authors	:	Wang, X.; Zhang, X.
Deposited on	:	1997-07-30
Resolution	:	2.80 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 (1)) were used in the production of this report:

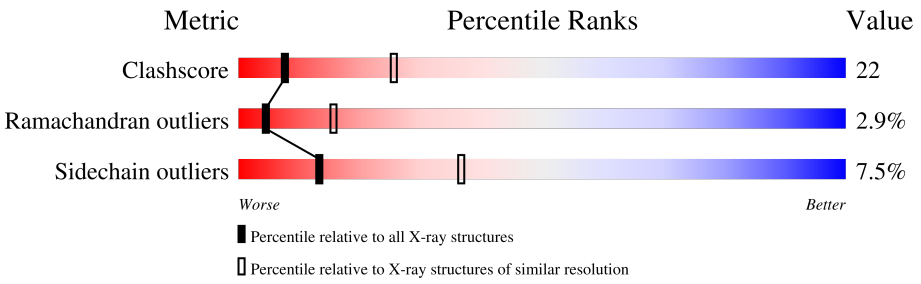
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	532	54% 41% 5%
1	B	532	55% 42% .

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	TCH	A	601	X	-	-	-
3	TCH	A	602	X	-	-	-
3	TCH	B	601	X	-	-	-
3	TCH	B	602	X	-	-	-

2 Entry composition (i)

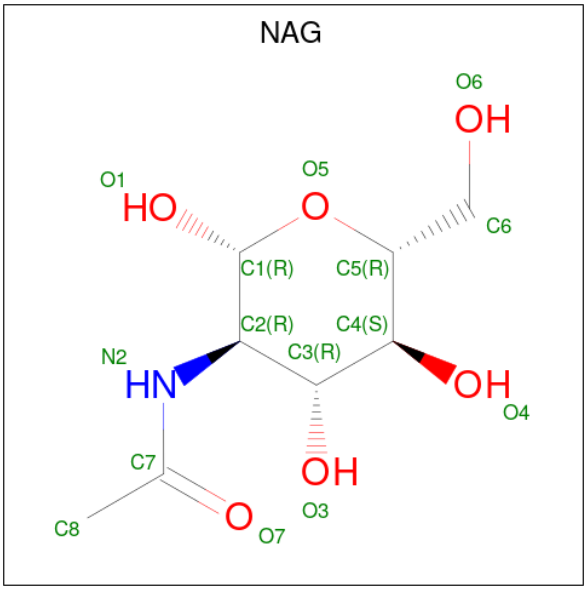
There are 3 unique types of molecules in this entry. The entry contains 8498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BILE-SALT ACTIVATED LIPASE.

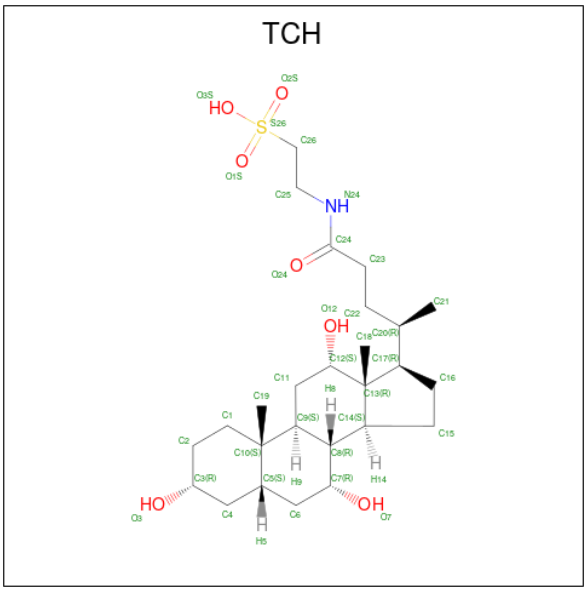
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4165	2668	692	788	17	0	0	0
1	B	532	4165	2668	692	788	17	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0

- Molecule 3 is TAUROCHOLIC ACID (three-letter code: TCH) (formula: $C_{26}H_{45}NO_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	35	26	1	7	1	0	0
			Total	C	N	O	S		
3	A	1	35	26	1	7	1	0	0
			Total	C	N	O	S		
3	B	1	35	26	1	7	1	0	0
			Total	C	N	O	S		
3	B	1	35	26	1	7	1	0	0

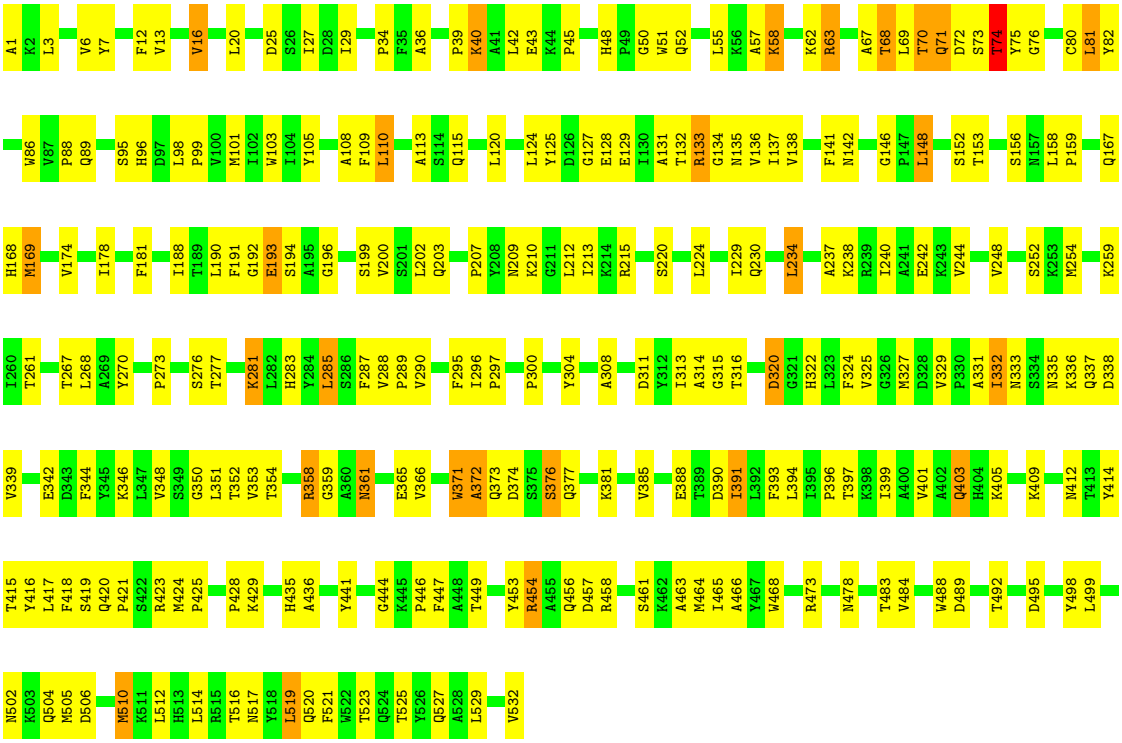
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: BILE-SALT ACTIVATED LIPASE

Chain A: 54% 41% 5%



• Molecule 1: BILE-SALT ACTIVATED LIPASE

Chain B: 55% 42% •

I291
D294 F295 I296 P297 D298 D299 P300 V301 N302 L303 Y304
A308 D309 V310
I313 A314
D318 M319 D320 G321 H322
V325
P330 A331 I332 N333 S334 N335 K336 Q337 D338 V339 T340 E341 E342 D343
K346
G350 L351 T352
K355 G356 L357 R358 G359 A360 N361 A362 T363 Y364
E365
E369 P370 W371 A372 Q373 D374
Q377
R380 K381 K382 T383 M384 V385 D386 L387 E388 T389 D390 I391 L392 F393 L394 I395 P396 T397 K398 I399 A400 V401
H404
A408 K409
N412 T413 Y414 T415 Y416 L417
R423 M424
Y427 P428 K429 W430 M431
H435 A436 D437 D438 L439
Q440 Y441 V442 F443 G444 K445 P446 F447 A448 T449 P450 L451 G452 Y453 R454 A455 Q456 D457 R458 T459 V460 S461 K462
I465
W468 T469
R473 T474
T483
D489 P490
E494 D495 D496 N497 Y498
K503 Q504
S507
M510 K511 L512 H513 L514 R515
L519 Q520 F521 W522
T525 Y526 Q527
P530 T531 V532

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	130.23Å 104.09Å 120.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	79.5 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.211 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

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: TCH, NAG

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	0.46	0/4278	0.71	0/5824
1	B	0.44	0/4278	0.69	1/5824 (0.0%)
All	All	0.45	0/8556	0.70	1/11648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	LEU	CA-CB-CG	5.61	128.19	115.30

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	4165	0	4055	196	0
1	B	4165	0	4055	170	0
2	A	14	0	13	2	0
2	B	14	0	13	1	0
3	A	70	0	82	9	0
3	B	70	0	82	11	0
All	All	8498	0	8300	369	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 22.

All (369) 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:67:ALA:HA	1:B:73:SER:HA	1.37	1.04
1:B:115:GLN:H	1:B:115:GLN:HE21	1.11	0.96
1:B:325:VAL:HB	1:B:388:GLU:HG3	1.50	0.92
1:A:336:LYS:HG3	1:A:337:GLN:H	1.34	0.92
1:A:336:LYS:HE2	1:A:337:GLN:HG2	1.52	0.91
1:A:148:LEU:HD11	1:A:267:THR:OG1	1.73	0.88
1:B:399:ILE:HD13	3:B:602:TCH:H19B	1.59	0.84
1:A:342:GLU:HG2	1:A:346:LYS:HE3	1.60	0.81
1:A:418:PHE:HE1	1:A:464:MET:SD	2.02	0.81
1:A:336:LYS:HD3	1:B:451:LEU:HD22	1.63	0.80
1:A:351:LEU:HD13	1:A:391:ILE:HD11	1.66	0.76
1:A:313:ILE:HG12	1:A:414:TYR:HB2	1.68	0.75
1:A:99:PRO:HB2	1:A:136:VAL:HG23	1.67	0.75
1:B:295:PHE:O	1:B:297:PRO:HD3	1.85	0.75
1:A:295:PHE:O	1:A:297:PRO:HD3	1.88	0.74
1:B:283:HIS:HE1	1:B:350:GLY:O	1.71	0.73
1:B:449:THR:HG21	3:B:601:TCH:O7	1.89	0.72
1:A:62:LYS:HG3	1:A:76:GLY:HA2	1.69	0.72
1:B:118:ASN:HA	1:B:122:ASN:O	1.89	0.72
1:A:148:LEU:HD12	1:A:148:LEU:H	1.55	0.72
1:B:357:LEU:HA	1:B:360:ALA:HB3	1.71	0.72
1:A:196:GLY:O	1:A:200:VAL:HG23	1.89	0.71
1:A:372:ALA:HB1	1:A:376:SER:HB2	1.73	0.71
1:B:447:PHE:O	1:B:450:PRO:HD3	1.90	0.71
1:B:374:ASP:HA	1:B:380:ARG:HH22	1.55	0.71
1:B:288:VAL:HB	1:B:289:PRO:HD2	1.72	0.70
3:B:602:TCH:H7	3:B:602:TCH:H19	1.71	0.70
1:A:67:ALA:HA	1:A:73:SER:HA	1.73	0.69
1:B:445:LYS:O	1:B:449:THR:HG22	1.93	0.69
1:A:127:GLY:HA3	1:A:138:VAL:HG11	1.73	0.68
1:A:16:VAL:HG22	1:A:29:ILE:HB	1.76	0.68
1:A:351:LEU:O	3:A:602:TCH:H25A	1.93	0.68
1:A:399:ILE:O	1:A:403:GLN:HB2	1.94	0.67
1:A:391:ILE:HG22	3:A:602:TCH:H21	1.77	0.67
1:A:40:LYS:O	1:A:43:GLU:HB2	1.95	0.66
1:A:361:ASN:HB3	2:A:600:NAG:H2	1.77	0.66
1:A:418:PHE:CE1	1:A:464:MET:SD	2.85	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:THR:O	1:B:401:VAL:HG23	1.96	0.66
1:A:336:LYS:HG3	1:A:337:GLN:N	2.10	0.66
1:B:115:GLN:H	1:B:115:GLN:NE2	1.89	0.66
1:B:230:GLN:HB3	1:B:290:VAL:HG12	1.77	0.66
1:B:273:PRO:HG2	1:B:284:TYR:CD2	2.30	0.66
1:B:115:GLN:HE21	1:B:115:GLN:N	1.89	0.65
1:A:338:ASP:HA	1:A:381:LYS:HZ3	1.61	0.65
1:A:396:PRO:HG3	3:A:602:TCH:H16	1.79	0.65
1:A:68:THR:HB	1:A:71:GLN:OE1	1.96	0.65
1:B:338:ASP:HB2	1:B:377:GLN:NE2	2.12	0.65
1:B:222:VAL:HG21	1:B:400:ALA:CB	2.28	0.64
1:B:495:ASP:HB3	1:B:512:LEU:HD22	1.79	0.64
1:A:361:ASN:CB	2:A:600:NAG:H2	2.28	0.64
1:B:374:ASP:HA	1:B:380:ARG:NH2	2.12	0.64
1:A:40:LYS:HB2	1:A:43:GLU:HB2	1.80	0.64
1:A:374:ASP:O	1:A:377:GLN:HG2	1.98	0.64
1:A:270:TYR:CG	1:A:287:PHE:HE2	2.17	0.63
1:A:478:ASN:HA	1:A:484:VAL:HG11	1.80	0.63
1:B:264:ARG:HD2	1:B:264:ARG:N	2.14	0.63
1:B:168:HIS:HD2	1:B:209:ASN:OD1	1.80	0.63
1:B:424:MET:HG2	1:B:427:TYR:CD1	2.34	0.63
1:A:409:LYS:NZ	1:A:409:LYS:HB3	2.13	0.63
1:B:503:LYS:HG3	1:B:504:GLN:HG3	1.81	0.62
1:A:333:ASN:ND2	1:A:335:ASN:HB3	2.15	0.62
1:A:320:ASP:O	1:A:435:HIS:HB2	2.00	0.61
1:A:325:VAL:HB	1:A:388:GLU:HG3	1.83	0.61
1:A:333:ASN:OD1	1:A:336:LYS:HG3	2.00	0.61
1:B:24:GLY:HA3	1:B:91:ARG:HB3	1.83	0.61
1:A:446:PRO:HA	1:A:453:TYR:CD2	2.35	0.61
1:A:489:ASP:HB2	1:A:510:MET:SD	2.41	0.61
1:A:381:LYS:O	1:A:385:VAL:HG23	2.00	0.61
1:A:374:ASP:HA	1:A:377:GLN:OE1	2.01	0.60
1:A:454:ARG:HB2	1:A:456:GLN:OE1	2.02	0.60
1:B:456:GLN:O	1:B:460:VAL:HG23	2.02	0.60
1:B:230:GLN:HE21	1:B:232:ASP:H	1.48	0.60
1:A:230:GLN:HB3	1:A:290:VAL:HG12	1.83	0.60
1:A:391:ILE:CB	3:A:602:TCH:H21	2.32	0.60
1:A:495:ASP:HB3	1:A:512:LEU:HD23	1.84	0.59
1:A:332:ILE:HG23	1:A:428:PRO:HD3	1.84	0.59
1:B:39:PRO:HB2	1:B:144:ARG:NH1	2.18	0.59
1:B:264:ARG:HD2	1:B:264:ARG:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:GLN:HB3	1:B:380:ARG:NH2	2.17	0.59
1:A:129:GLU:HG2	1:A:444:GLY:HA3	1.84	0.59
1:A:449:THR:HG23	1:A:453:TYR:HE2	1.67	0.58
1:A:73:SER:H	1:A:268:LEU:HD11	1.68	0.58
1:A:16:VAL:CG2	1:A:29:ILE:HB	2.34	0.58
1:A:108:ALA:O	1:A:109:PHE:HB2	2.05	0.57
1:A:108:ALA:HB3	1:A:110:LEU:CD2	2.34	0.57
1:A:391:ILE:CG2	3:A:602:TCH:H21	2.33	0.57
1:A:416:TYR:HB3	1:A:488:TRP:CZ2	2.39	0.57
1:A:498:TYR:CE1	1:A:514:LEU:HB2	2.39	0.57
1:A:74:THR:O	1:A:75:TYR:HD1	1.87	0.57
1:B:165:TRP:HH2	1:B:208:TYR:CZ	2.23	0.57
1:A:141:PHE:CE2	1:A:167:GLN:HA	2.39	0.57
1:A:199:SER:O	1:A:203:GLN:HG2	2.05	0.57
1:A:316:THR:O	1:A:417:LEU:HD12	2.05	0.57
1:B:218:SER:O	1:B:314:ALA:HA	2.05	0.57
1:B:155:ASP:OD2	1:B:251:THR:HG21	2.04	0.57
1:A:397:THR:O	1:A:401:VAL:HG23	2.05	0.56
1:A:463:ALA:O	1:A:466:ALA:HB3	2.04	0.56
1:B:3:LEU:HD21	1:B:181:PHE:HA	1.87	0.56
1:B:444:GLY:CA	1:B:465:ILE:HD11	2.35	0.56
1:A:308:ALA:HB1	1:A:409:LYS:HG3	1.87	0.56
1:B:224:LEU:HD22	1:B:301:VAL:HG12	1.86	0.56
1:B:498:TYR:CZ	1:B:511:LYS:HB2	2.41	0.56
1:B:313:ILE:HG12	1:B:414:TYR:HB2	1.87	0.55
1:A:110:LEU:HA	1:A:146:GLY:H	1.72	0.55
1:B:230:GLN:HE21	1:B:231:GLN:N	2.05	0.55
3:B:602:TCH:H19	3:B:602:TCH:C7	2.34	0.55
1:A:73:SER:HB2	1:A:268:LEU:HG	1.88	0.55
1:A:372:ALA:HB1	1:A:376:SER:CB	2.36	0.55
1:B:196:GLY:O	1:B:200:VAL:HG23	2.07	0.55
1:B:494:GLU:O	1:B:513:HIS:HE1	1.89	0.55
1:B:438:ASP:O	1:B:442:VAL:HG23	2.07	0.54
1:B:401:VAL:HG11	1:B:415:THR:HB	1.88	0.54
1:A:193:GLU:OE2	1:A:436:ALA:HA	2.06	0.54
1:A:344:PHE:O	1:A:348:VAL:HG23	2.07	0.54
1:B:135:ASN:HB3	1:B:473:ARG:NH2	2.23	0.54
1:B:358:ARG:CZ	1:B:530:PRO:HG2	2.38	0.54
1:A:391:ILE:HB	3:A:602:TCH:H21	1.90	0.54
1:B:382:LYS:HE2	1:B:430:TRP:HB2	1.88	0.54
1:B:291:ILE:HG23	1:B:296:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:HB2	1:B:377:GLN:HE22	1.71	0.54
1:A:63:ARG:HE	1:A:113:ALA:HB2	1.73	0.53
3:B:601:TCH:H18B	3:B:601:TCH:H22	1.89	0.53
1:A:358:ARG:CG	1:A:529:LEU:HD13	2.38	0.53
1:A:153:THR:O	1:A:234:LEU:HD22	2.09	0.53
1:B:190:LEU:HB2	1:B:213:ILE:HD12	1.90	0.53
1:A:108:ALA:HB3	1:A:110:LEU:HD22	1.90	0.53
1:A:42:LEU:HB3	1:A:158:LEU:HD11	1.91	0.53
1:A:229:ILE:HD13	1:A:289:PRO:HB2	1.90	0.53
1:B:222:VAL:HG21	1:B:400:ALA:HB1	1.90	0.53
1:A:333:ASN:C	1:A:335:ASN:H	2.13	0.52
1:A:40:LYS:H	1:A:40:LYS:HD2	1.72	0.52
1:B:174:VAL:O	1:B:178:ILE:HB	2.09	0.52
1:B:272:LEU:HD23	1:B:273:PRO:HD2	1.90	0.52
1:B:449:THR:HG23	1:B:449:THR:O	2.08	0.52
1:B:522:TRP:O	1:B:527:GLN:HG2	2.09	0.52
1:A:495:ASP:HB3	1:A:512:LEU:CD2	2.39	0.52
1:B:449:THR:CG2	3:B:601:TCH:H15	2.39	0.52
1:B:134:GLY:HA3	1:B:469:THR:HG21	1.91	0.52
1:A:96:HIS:O	1:A:98:LEU:HD12	2.10	0.52
1:B:322:HIS:CD2	1:B:431:MET:SD	3.03	0.52
1:A:133:ARG:NH2	1:A:447:PHE:CG	2.78	0.52
1:B:191:PHE:HB2	1:B:217:ILE:HB	1.90	0.51
1:A:128:GLU:O	1:A:132:THR:HG23	2.11	0.51
1:A:95:SER:HB3	1:A:98:LEU:CD1	2.41	0.51
1:A:27:ILE:HD12	1:A:88:PRO:HA	1.92	0.51
1:A:234:LEU:HD12	1:A:234:LEU:O	2.11	0.51
1:B:230:GLN:NE2	1:B:232:ASP:H	2.08	0.51
1:B:125:TYR:HA	1:B:443:PHE:CD2	2.46	0.51
1:B:235:PHE:O	1:B:239:ARG:HG2	2.11	0.51
1:A:103:TRP:CZ3	1:A:192:GLY:HA2	2.45	0.51
1:B:391:ILE:HG13	1:B:392:LEU:N	2.26	0.51
1:A:48:HIS:HD2	1:A:50:GLY:H	1.57	0.50
1:B:118:ASN:HB3	1:B:123:TYR:CD1	2.46	0.50
1:B:158:LEU:HD12	1:B:162:TYR:OH	2.11	0.50
1:B:458:ARG:O	1:B:462:LYS:HB2	2.10	0.50
1:B:199:SER:O	1:B:203:GLN:HG2	2.10	0.50
1:B:342:GLU:HG3	1:B:343:ASP:N	2.25	0.50
1:B:394:LEU:O	1:B:398:LYS:HG2	2.12	0.50
1:A:220:SER:HB3	1:A:435:HIS:CE1	2.46	0.50
1:B:273:PRO:HG2	1:B:284:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:VAL:HG11	1:B:385:VAL:HG22	1.94	0.50
1:A:168:HIS:CD2	1:A:209:ASN:OD1	2.65	0.50
1:A:366:VAL:HG11	1:A:521:PHE:CZ	2.46	0.50
1:A:405:LYS:NZ	1:A:492:THR:HA	2.27	0.50
1:B:150:PHE:HE1	1:B:164:LEU:HD23	1.76	0.50
1:B:190:LEU:O	1:B:216:ALA:HA	2.12	0.50
1:A:288:VAL:HB	1:A:289:PRO:CD	2.42	0.50
1:B:167:GLN:OE1	1:B:199:SER:HB3	2.12	0.49
1:A:51:TRP:NE1	1:A:55:LEU:HB2	2.28	0.49
1:B:70:THR:HB	1:B:271:LYS:HG3	1.95	0.49
1:B:446:PRO:HG3	1:B:453:TYR:CD2	2.47	0.49
1:A:3:LEU:HD21	1:A:181:PHE:HA	1.95	0.49
1:B:495:ASP:HB3	1:B:512:LEU:CD2	2.40	0.49
1:B:449:THR:OG1	3:B:601:TCH:H15	2.13	0.49
1:A:281:LYS:H	1:A:281:LYS:HD3	1.78	0.49
1:A:315:GLY:HA3	1:A:416:TYR:CE2	2.48	0.49
1:B:157:ASN:O	1:B:158:LEU:HB2	2.13	0.49
1:B:298:ASP:OD1	1:B:302:ASN:HB2	2.13	0.49
1:B:361:ASN:CB	2:B:600:NAG:H2	2.43	0.48
1:A:194:SER:OG	1:A:435:HIS:NE2	2.46	0.48
1:A:461:SER:O	1:A:465:ILE:HG13	2.13	0.48
1:A:488:TRP:CD2	1:A:499:LEU:HD22	2.48	0.48
1:B:150:PHE:HE1	1:B:164:LEU:CD2	2.26	0.48
1:B:412:ASN:HB3	1:B:414:TYR:CE1	2.48	0.48
1:B:338:ASP:HB2	1:B:377:GLN:CD	2.34	0.48
1:B:377:GLN:HB3	1:B:380:ARG:HH21	1.78	0.48
1:B:300:PRO:HA	1:B:303:LEU:HD12	1.96	0.48
1:B:175:LYS:HG2	1:B:212:LEU:HD22	1.96	0.48
1:B:200:VAL:CG1	1:B:216:ALA:HB1	2.43	0.48
1:B:435:HIS:O	1:B:436:ALA:HB3	2.13	0.48
1:B:514:LEU:HG	1:B:515:ARG:HG2	1.95	0.48
1:B:363:THR:HA	1:B:521:PHE:CZ	2.49	0.47
1:B:152:SER:HA	1:B:158:LEU:O	2.14	0.47
1:A:338:ASP:HA	1:A:381:LYS:NZ	2.29	0.47
1:B:355:LYS:HG3	1:B:530:PRO:O	2.15	0.47
1:B:164:LEU:HD21	1:B:289:PRO:HB3	1.96	0.47
1:A:34:PRO:HB3	1:A:82:TYR:CE2	2.49	0.47
1:A:124:LEU:O	1:A:125:TYR:HD1	1.98	0.47
1:B:298:ASP:H	1:B:303:LEU:HD21	1.79	0.47
1:A:396:PRO:HG3	3:A:602:TCH:C16	2.45	0.47
1:B:454:ARG:O	1:B:457:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PRO:HG2	1:A:461:SER:HB2	1.96	0.47
1:B:152:SER:O	1:B:237:ALA:HB2	2.15	0.47
1:A:108:ALA:HB1	1:A:285:LEU:HD21	1.97	0.47
1:A:120:LEU:N	1:A:120:LEU:HD22	2.30	0.47
1:B:127:GLY:HA3	1:B:138:VAL:HG11	1.96	0.47
1:B:135:ASN:O	1:B:473:ARG:NH2	2.48	0.47
1:B:380:ARG:HA	1:B:383:THR:OG1	2.15	0.47
1:B:152:SER:HB2	1:B:160:GLY:HA3	1.95	0.47
1:A:81:LEU:N	1:A:81:LEU:HD23	2.30	0.46
1:A:86:TRP:O	1:A:137:ILE:HG23	2.16	0.46
1:A:339:VAL:H	1:A:381:LYS:HZ1	1.63	0.46
1:B:92:LYS:HE2	1:B:93:GLU:HG2	1.96	0.46
1:B:224:LEU:HD21	1:B:304:TYR:HE1	1.80	0.46
1:A:13:VAL:CG1	1:A:57:ALA:HB2	2.46	0.46
1:A:68:THR:HG22	1:A:69:LEU:H	1.80	0.46
1:A:105:TYR:HE2	1:A:142:ASN:HA	1.81	0.46
1:A:242:GLU:HG2	1:A:248:VAL:HG11	1.97	0.46
1:A:314:ALA:O	1:A:415:THR:HA	2.16	0.46
1:A:339:VAL:H	1:A:381:LYS:NZ	2.14	0.46
1:A:20:LEU:HD11	1:A:27:ILE:HB	1.97	0.46
1:B:204:THR:HG21	1:B:310:VAL:HG11	1.97	0.46
1:B:449:THR:HG21	3:B:601:TCH:HO7	1.81	0.46
1:A:62:LYS:HD2	1:A:62:LYS:HA	1.69	0.46
1:A:68:THR:HG23	1:A:75:TYR:CZ	2.51	0.46
1:B:342:GLU:O	1:B:346:LYS:HG3	2.16	0.46
1:A:131:ALA:HB2	1:A:138:VAL:HG23	1.98	0.46
1:A:42:LEU:HB2	1:A:259:LYS:HG2	1.98	0.46
1:A:418:PHE:CE2	1:A:420:GLN:HB3	2.51	0.46
1:A:519:LEU:O	1:A:523:THR:HG23	2.16	0.46
1:A:424:MET:HA	1:A:425:PRO:HD2	1.79	0.45
1:A:371:TRP:HE3	1:A:371:TRP:O	1.98	0.45
1:A:72:ASP:HB3	1:A:74:THR:OG1	2.16	0.45
1:B:497:ASN:HB3	1:B:512:LEU:CD2	2.47	0.45
1:B:224:LEU:HD21	1:B:304:TYR:CE1	2.52	0.45
1:A:331:ALA:O	1:A:333:ASN:N	2.49	0.45
1:B:27:ILE:CD1	1:B:128:GLU:HG3	2.46	0.45
1:B:369:GLU:N	1:B:370:PRO:HD2	2.32	0.45
1:B:424:MET:HG2	1:B:427:TYR:CE1	2.51	0.45
1:A:40:LYS:HB2	1:A:43:GLU:CB	2.46	0.45
1:A:324:PHE:CE2	1:A:393:PHE:HZ	2.35	0.45
1:A:517:ASN:O	1:A:520:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:HD11	1:B:174:VAL:HG11	1.98	0.45
3:B:601:TCH:H22	3:B:601:TCH:C18	2.46	0.45
1:A:188:ILE:HD12	1:A:212:LEU:O	2.17	0.45
1:A:361:ASN:OD1	1:A:361:ASN:N	2.50	0.45
1:B:232:ASP:N	1:B:233:PRO:HD3	2.32	0.45
1:B:240:ILE:O	1:B:244:VAL:HG22	2.17	0.45
1:A:39:PRO:HD3	1:A:81:LEU:HG	1.99	0.44
1:A:449:THR:HG23	1:A:453:TYR:CE2	2.50	0.44
1:A:449:THR:O	1:A:453:TYR:HD2	2.01	0.44
1:B:177:ASN:N	1:B:177:ASN:ND2	2.65	0.44
1:B:497:ASN:HA	1:B:512:LEU:HD23	1.98	0.44
1:B:498:TYR:CE1	1:B:511:LYS:HB2	2.52	0.44
1:A:13:VAL:HG13	1:A:55:LEU:HD22	1.98	0.44
1:A:336:LYS:HD3	1:B:451:LEU:HA	1.99	0.44
3:B:602:TCH:H11A	3:B:602:TCH:H1A	1.76	0.44
1:B:167:GLN:O	1:B:171:ILE:HG13	2.17	0.44
1:B:314:ALA:O	1:B:415:THR:HA	2.17	0.44
1:B:404:HIS:O	1:B:408:ALA:HB2	2.18	0.44
1:A:202:LEU:HD22	1:A:296:ILE:HD12	2.00	0.44
1:A:342:GLU:O	1:A:346:LYS:HG3	2.17	0.44
1:B:48:HIS:CG	1:B:49:PRO:HD2	2.52	0.44
1:B:489:ASP:HB2	1:B:510:MET:HE2	1.99	0.44
1:A:95:SER:HB3	1:A:98:LEU:HD13	2.00	0.44
1:A:238:LYS:HA	1:A:254:MET:CE	2.47	0.44
1:A:488:TRP:CE3	1:A:499:LEU:HD22	2.53	0.44
1:B:191:PHE:CB	1:B:217:ILE:HB	2.47	0.44
1:B:325:VAL:CB	1:B:388:GLU:HG3	2.35	0.44
1:A:224:LEU:HD23	1:A:300:PRO:HB2	2.00	0.44
1:A:333:ASN:HD21	1:A:335:ASN:HB3	1.83	0.44
1:A:419:SER:O	1:A:421:PRO:HD3	2.17	0.44
1:A:399:ILE:HD12	3:A:602:TCH:H15A	2.00	0.44
1:B:218:SER:HB3	1:B:221:GLY:O	2.18	0.44
1:B:279:TYR:CD1	1:B:279:TYR:N	2.85	0.44
1:A:7:TYR:HB2	1:A:12:PHE:CE1	2.53	0.44
1:A:101:MET:HB3	1:A:191:PHE:CE1	2.53	0.44
1:A:133:ARG:NH2	1:A:447:PHE:CD2	2.86	0.44
1:A:366:VAL:HG11	1:A:521:PHE:CE1	2.52	0.44
1:B:16:VAL:O	1:B:28:ASP:HA	2.18	0.43
1:A:456:GLN:CD	1:A:456:GLN:H	2.22	0.43
1:B:62:LYS:HA	1:B:62:LYS:HD3	1.80	0.43
1:B:340:THR:O	1:B:343:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ASP:HA	1:B:417:LEU:HD11	2.00	0.43
1:B:361:ASN:O	1:B:365:GLU:HG3	2.19	0.43
1:A:1:ALA:HB3	1:A:89:GLN:HB3	1.99	0.43
1:A:359:GLY:HA2	1:A:529:LEU:HD12	2.00	0.43
1:A:371:TRP:CD2	1:A:371:TRP:N	2.86	0.43
1:B:208:TYR:HE2	1:B:294:ASP:HB2	1.82	0.43
1:B:497:ASN:HB3	1:B:512:LEU:HD23	2.00	0.43
1:B:332:ILE:HD13	1:B:332:ILE:H	1.83	0.43
1:A:131:ALA:O	1:A:135:ASN:N	2.47	0.43
1:A:158:LEU:N	1:A:159:PRO:HD3	2.33	0.43
1:A:458:ARG:NH1	1:A:458:ARG:HG3	2.34	0.43
1:B:147:PRO:HG2	1:B:267:THR:HA	2.00	0.43
1:A:40:LYS:H	1:A:40:LYS:CD	2.32	0.43
1:A:337:GLN:CG	1:B:451:LEU:HD21	2.48	0.43
1:B:108:ALA:HB3	1:B:110:LEU:HD23	2.00	0.43
1:B:243:LYS:HE2	1:B:269:ALA:HA	2.00	0.43
1:B:451:LEU:HD22	1:B:451:LEU:HA	1.74	0.43
1:A:283:HIS:HE1	1:A:350:GLY:O	2.02	0.43
1:A:454:ARG:HD3	1:A:454:ARG:N	2.34	0.43
1:B:157:ASN:HD22	1:B:252:SER:HA	1.84	0.43
1:B:270:TYR:HB2	1:B:287:PHE:HE2	1.83	0.43
1:B:258:LEU:C	1:B:260:ILE:H	2.22	0.42
1:A:405:LYS:HZ2	1:A:492:THR:HA	1.82	0.42
1:A:167:GLN:HB2	1:A:203:GLN:NE2	2.33	0.42
1:A:242:GLU:CG	1:A:248:VAL:HG11	2.49	0.42
1:A:13:VAL:HG22	1:A:51:TRP:HZ2	1.83	0.42
1:B:190:LEU:HD22	1:B:213:ILE:HD11	2.01	0.42
1:B:222:VAL:HG22	1:B:223:GLY:H	1.84	0.42
1:B:313:ILE:HA	1:B:414:TYR:O	2.19	0.42
1:A:174:VAL:O	1:A:178:ILE:HB	2.19	0.42
1:A:352:THR:O	1:A:354:THR:N	2.52	0.42
1:A:358:ARG:HG3	1:A:529:LEU:HD13	2.00	0.42
1:B:73:SER:HB2	1:B:268:LEU:HG	2.02	0.42
1:A:58:LYS:HD3	1:A:58:LYS:C	2.39	0.42
1:A:207:PRO:HD2	1:A:295:PHE:O	2.20	0.42
1:A:420:GLN:HA	1:A:421:PRO:HD2	1.89	0.42
1:B:243:LYS:HE3	1:B:243:LYS:HB3	1.90	0.42
1:A:36:ALA:HB3	1:A:81:LEU:HD12	2.01	0.42
1:B:204:THR:CG2	1:B:310:VAL:HG11	2.50	0.42
1:B:40:LYS:O	1:B:41:ALA:C	2.57	0.42
1:A:215:ARG:HD3	1:A:311:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:OG	1:A:502:ASN:HB3	2.20	0.41
1:A:502:ASN:O	1:A:505:MET:HG2	2.20	0.41
1:B:386:ASP:O	1:B:390:ASP:OD2	2.38	0.41
1:A:238:LYS:O	1:A:242:GLU:HG3	2.19	0.41
1:A:333:ASN:C	1:A:335:ASN:N	2.72	0.41
1:B:230:GLN:HE21	1:B:231:GLN:H	1.67	0.41
1:B:333:ASN:ND2	1:B:337:GLN:OE1	2.53	0.41
1:A:193:GLU:O	1:A:196:GLY:N	2.52	0.41
1:A:320:ASP:OD1	1:A:435:HIS:HA	2.20	0.41
1:A:336:LYS:HD3	1:B:451:LEU:CD2	2.42	0.41
3:A:601:TCH:H1A	3:A:601:TCH:H11A	1.81	0.41
1:B:338:ASP:HB2	1:B:377:GLN:OE1	2.19	0.41
1:A:152:SER:O	1:A:237:ALA:HB2	2.21	0.41
1:A:190:LEU:HD23	1:A:213:ILE:HG12	2.02	0.41
1:A:336:LYS:HB2	1:A:336:LYS:HE3	1.85	0.41
1:B:230:GLN:OE1	1:B:236:TRP:CZ3	2.73	0.41
1:B:395:ILE:HG13	1:B:519:LEU:HD23	2.03	0.41
1:B:194:SER:O	1:B:197:GLY:N	2.54	0.41
1:B:105:TYR:HE2	1:B:142:ASN:HA	1.86	0.41
1:B:352:THR:HG22	1:B:526:TYR:CE2	2.56	0.41
1:A:240:ILE:O	1:A:244:VAL:HG22	2.20	0.41
1:A:390:ASP:HA	1:A:394:LEU:HB3	2.01	0.41
1:A:441:TYR:HE2	1:A:457:ASP:HA	1.85	0.41
1:B:489:ASP:HA	1:B:490:PRO:HD3	1.91	0.41
1:A:45:PRO:HG2	1:A:169:MET:CE	2.50	0.41
1:B:32:GLY:CA	1:B:61:LYS:HD3	2.51	0.41
1:B:115:GLN:HG2	1:B:116:GLY:N	2.36	0.41
1:B:308:ALA:HB1	1:B:409:LYS:HB2	2.03	0.41
1:A:63:ARG:HA	1:A:142:ASN:ND2	2.36	0.40
1:A:429:LYS:HB2	1:A:429:LYS:NZ	2.36	0.40
1:A:20:LEU:HB2	1:A:25:ASP:O	2.21	0.40
1:A:88:PRO:HG3	1:A:131:ALA:HB1	2.02	0.40
1:A:315:GLY:HA3	1:A:416:TYR:CD2	2.56	0.40
1:B:239:ARG:HH11	1:B:239:ARG:HA	1.86	0.40
1:B:243:LYS:CE	1:B:269:ALA:HA	2.51	0.40
1:B:440:GLN:CG	1:B:441:TYR:N	2.84	0.40
1:A:134:GLY:O	1:A:473:ARG:NH2	2.54	0.40
1:A:401:VAL:HG11	1:A:415:THR:HB	2.04	0.40
1:A:412:ASN:HB2	1:A:414:TYR:HE1	1.87	0.40
3:B:601:TCH:H19	3:B:601:TCH:H6A	1.94	0.40
1:B:332:ILE:O	1:B:428:PRO:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:CZ	1:A:447:PHE:CD2	3.05	0.40
1:A:220:SER:HB3	1:A:435:HIS:HE1	1.86	0.40
1:A:322:HIS:NE2	1:A:332:ILE:HG12	2.36	0.40
1:A:358:ARG:HG2	1:A:529:LEU:HD13	2.03	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	530/532 (100%)	451 (85%)	63 (12%)	16 (3%)	4 15
1	B	530/532 (100%)	456 (86%)	59 (11%)	15 (3%)	5 17
All	All	1060/1064 (100%)	907 (86%)	122 (12%)	31 (3%)	4 15

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	VAL
1	B	52	GLN
1	B	68	THR
1	B	158	LEU
1	A	70	THR
1	A	156	SER
1	A	281	LYS
1	A	332	ILE
1	B	210	LYS
1	A	80	CYS
1	A	210	LYS
1	A	276	SER
1	A	304	TYR
1	A	372	ALA

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Mol	Chain	Res	Type
1	A	373	GLN
1	B	259	LYS
1	B	297	PRO
1	B	335	ASN
1	B	525	THR
1	A	74	THR
1	A	273	PRO
1	A	525	THR
1	B	70	THR
1	B	148	LEU
1	B	228	ALA
1	B	372	ALA
1	A	16	VAL
1	A	68	THR
1	B	513	HIS
1	B	107	GLY
1	B	330	PRO

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	444/444 (100%)	403 (91%)	41 (9%)	9 27
1	B	444/444 (100%)	418 (94%)	26 (6%)	19 49
All	All	888/888 (100%)	821 (92%)	67 (8%)	13 37

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	40	LYS
1	A	52	GLN
1	A	58	LYS
1	A	63	ARG
1	A	70	THR

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	74	THR
1	A	81	LEU
1	A	110	LEU
1	A	115	GLN
1	A	133	ARG
1	A	148	LEU
1	A	169	MET
1	A	193	GLU
1	A	234	LEU
1	A	252	SER
1	A	261	THR
1	A	277	THR
1	A	285	LEU
1	A	320	ASP
1	A	327	MET
1	A	329	VAL
1	A	358	ARG
1	A	361	ASN
1	A	365	GLU
1	A	371	TRP
1	A	376	SER
1	A	391	ILE
1	A	403	GLN
1	A	423	ARG
1	A	454	ARG
1	A	468	TRP
1	A	483	THR
1	A	504	GLN
1	A	506	ASP
1	A	510	MET
1	A	516	THR
1	A	519	LEU
1	A	527	GLN
1	A	532	VAL
1	B	16	VAL
1	B	68	THR
1	B	71	GLN
1	B	74	THR
1	B	110	LEU
1	B	115	GLN
1	B	177	ASN

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Mol	Chain	Res	Type
1	B	194	SER
1	B	201	SER
1	B	234	LEU
1	B	235	PHE
1	B	250	ASP
1	B	263	PRO
1	B	282	LEU
1	B	300	PRO
1	B	320	ASP
1	B	332	ILE
1	B	383	THR
1	B	423	ARG
1	B	451	LEU
1	B	468	TRP
1	B	474	THR
1	B	483	THR
1	B	507	SER
1	B	519	LEU
1	B	530	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	168	HIS
1	A	230	GLN
1	A	231	GLN
1	A	283	HIS
1	A	520	GLN
1	A	524	GLN
1	B	17	ASN
1	B	115	GLN
1	B	157	ASN
1	B	168	HIS
1	B	177	ASN
1	B	230	GLN
1	B	283	HIS
1	B	513	HIS
1	B	520	GLN

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)

6 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	NAG	B	600	1	14,14,15	0.74	0	17,19,21	1.10	2 (11%)
2	NAG	A	600	1	14,14,15	0.72	0	17,19,21	0.97	2 (11%)
3	TCH	A	601	-	38,38,38	2.15	14 (36%)	59,60,60	4.58	37 (62%)
3	TCH	B	601	-	38,38,38	2.15	13 (34%)	59,60,60	4.56	35 (59%)
3	TCH	A	602	-	38,38,38	2.26	15 (39%)	59,60,60	4.70	34 (57%)
3	TCH	B	602	-	38,38,38	2.00	10 (26%)	59,60,60	4.47	35 (59%)

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	NAG	B	600	1	-	2/6/23/26	0/1/1/1
3	TCH	B	601	-	4/4/13/14	10/16/81/81	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TCH	A	601	-	4/4/13/14	9/16/81/81	0/4/4/4
2	NAG	A	600	1	-	2/6/23/26	0/1/1/1
3	TCH	A	602	-	4/4/13/14	8/16/81/81	0/4/4/4
3	TCH	B	602	-	4/4/13/14	11/16/81/81	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	TCH	C6-C5	-5.70	1.44	1.53
3	A	602	TCH	C6-C5	-5.46	1.45	1.53
3	A	602	TCH	C10-C5	-5.24	1.46	1.55
3	A	601	TCH	C8-C9	4.92	1.63	1.53
3	B	602	TCH	C11-C9	-4.67	1.46	1.53
3	B	602	TCH	C10-C5	-4.62	1.47	1.55
3	B	602	TCH	C10-C9	-4.44	1.47	1.56
3	B	601	TCH	C11-C12	4.43	1.60	1.53
3	A	602	TCH	C11-C9	-4.13	1.46	1.53
3	A	601	TCH	C20-C17	4.13	1.61	1.54
3	B	601	TCH	C10-C5	-4.08	1.48	1.55
3	A	602	TCH	C6-C7	-4.01	1.45	1.52
3	A	602	TCH	C8-C7	-3.98	1.46	1.53
3	B	602	TCH	C18-C13	3.85	1.60	1.54
3	A	601	TCH	C18-C13	3.84	1.60	1.54
3	B	601	TCH	C11-C9	-3.68	1.47	1.53
3	A	601	TCH	C11-C9	-3.56	1.47	1.53
3	A	601	TCH	O24-C24	3.51	1.30	1.23
3	A	601	TCH	C10-C5	-3.40	1.49	1.55
3	A	602	TCH	C21-C20	-3.28	1.45	1.53
3	A	602	TCH	O24-C24	3.20	1.29	1.23
3	B	601	TCH	C8-C9	3.17	1.60	1.53
3	B	602	TCH	C4-C3	3.06	1.57	1.51
3	B	602	TCH	C6-C7	3.00	1.58	1.52
3	A	601	TCH	C24-N24	2.96	1.40	1.33
3	B	601	TCH	C6-C7	-2.95	1.47	1.52
3	A	601	TCH	C13-C17	2.94	1.60	1.55
3	B	602	TCH	O24-C24	2.91	1.29	1.23
3	B	602	TCH	C8-C7	2.84	1.58	1.53
3	B	601	TCH	O24-C24	2.81	1.29	1.23
3	B	602	TCH	O12-C12	2.73	1.48	1.43
3	A	601	TCH	C8-C14	2.66	1.59	1.53
3	A	602	TCH	C18-C13	2.64	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	TCH	C18-C13	2.64	1.58	1.54
3	A	601	TCH	C6-C5	-2.62	1.49	1.53
3	A	602	TCH	C8-C14	-2.53	1.48	1.53
3	A	602	TCH	C10-C9	-2.49	1.51	1.56
3	B	601	TCH	C22-C23	2.36	1.60	1.52
3	A	602	TCH	C8-C9	2.34	1.58	1.53
3	A	602	TCH	C11-C12	2.33	1.57	1.53
3	B	602	TCH	C21-C20	-2.24	1.47	1.53
3	B	601	TCH	C26-S26	2.23	1.80	1.77
3	B	601	TCH	C2-C3	-2.20	1.46	1.51
3	B	601	TCH	C21-C20	-2.18	1.47	1.53
3	A	601	TCH	C11-C12	2.15	1.56	1.53
3	A	602	TCH	C26-S26	-2.14	1.74	1.77
3	A	602	TCH	C4-C5	-2.13	1.50	1.53
3	B	601	TCH	C19-C10	-2.12	1.50	1.54
3	A	601	TCH	C22-C23	2.09	1.59	1.52
3	A	601	TCH	C13-C12	2.07	1.57	1.54
3	A	602	TCH	C20-C17	-2.04	1.50	1.54
3	A	601	TCH	O12-C12	2.03	1.47	1.43

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	TCH	C15-C14-C13	14.85	118.12	103.55
3	B	601	TCH	C15-C14-C13	14.33	117.61	103.55
3	A	601	TCH	C15-C14-C13	13.77	117.06	103.55
3	B	602	TCH	C11-C9-C8	13.23	130.24	110.88
3	B	602	TCH	C15-C14-C13	13.02	116.33	103.55
3	A	601	TCH	C11-C9-C8	11.79	128.13	110.88
3	A	602	TCH	C11-C9-C8	11.60	127.86	110.88
3	B	601	TCH	C11-C9-C8	11.49	127.70	110.88
3	A	601	TCH	O2S-S26-C26	11.37	120.61	106.92
3	A	602	TCH	O2S-S26-C26	11.35	120.58	106.92
3	B	602	TCH	O2S-S26-C26	10.88	120.02	106.92
3	B	602	TCH	C9-C11-C12	-10.74	100.12	114.30
3	A	601	TCH	C9-C11-C12	-10.36	100.62	114.30
3	B	601	TCH	O2S-S26-C26	9.91	118.84	106.92
3	A	602	TCH	C9-C11-C12	-9.58	101.65	114.30
3	A	602	TCH	C5-C6-C7	-8.37	105.22	114.46
3	B	601	TCH	C9-C11-C12	-8.24	103.42	114.30
3	A	602	TCH	C10-C9-C8	7.91	120.31	111.82
3	B	601	TCH	C11-C12-C13	7.83	119.28	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	TCH	C10-C9-C8	7.73	120.12	111.82
3	B	602	TCH	O12-C12-C11	7.49	124.38	109.12
3	A	601	TCH	C18-C13-C12	7.48	116.68	109.07
3	B	601	TCH	O12-C12-C11	7.19	123.78	109.12
3	A	602	TCH	O12-C12-C11	7.08	123.55	109.12
3	A	602	TCH	C6-C5-C4	7.04	119.30	111.19
3	A	601	TCH	C10-C9-C8	6.88	119.20	111.82
3	A	602	TCH	C18-C13-C12	6.86	116.05	109.07
3	A	601	TCH	C13-C17-C20	6.72	127.52	119.50
3	B	601	TCH	O3-C3-C4	6.65	123.10	109.85
3	B	602	TCH	C15-C14-C8	6.55	127.49	118.33
3	A	601	TCH	O12-C12-C11	6.51	122.39	109.12
3	A	602	TCH	O3-C3-C4	6.46	122.72	109.85
3	A	601	TCH	O3-C3-C4	6.44	122.68	109.85
3	B	601	TCH	C16-C17-C13	6.34	109.77	103.55
3	B	601	TCH	C5-C6-C7	-6.18	107.64	114.46
3	A	601	TCH	C11-C12-C13	6.18	117.59	111.24
3	B	601	TCH	C18-C13-C12	6.10	115.28	109.07
3	A	601	TCH	C15-C14-C8	6.10	126.86	118.33
3	B	602	TCH	C18-C13-C12	6.09	115.27	109.07
3	A	602	TCH	C11-C12-C13	6.00	117.41	111.24
3	B	602	TCH	O3-C3-C4	5.98	121.76	109.85
3	B	602	TCH	C17-C13-C14	-5.88	94.17	100.09
3	B	601	TCH	C6-C5-C4	5.84	117.91	111.19
3	A	602	TCH	C13-C17-C20	5.77	126.38	119.50
3	A	602	TCH	C16-C17-C13	5.69	109.13	103.55
3	A	602	TCH	C17-C13-C14	-5.62	94.43	100.09
3	B	601	TCH	C15-C14-C8	5.51	126.04	118.33
3	B	602	TCH	C6-C5-C4	5.44	117.46	111.19
3	A	601	TCH	C16-C17-C13	5.44	108.89	103.55
3	B	601	TCH	C13-C17-C20	5.40	125.94	119.50
3	B	601	TCH	C4-C3-C2	-5.30	104.22	110.55
3	B	602	TCH	C16-C17-C13	5.28	108.73	103.55
3	B	602	TCH	C14-C8-C7	5.26	118.78	111.81
3	B	601	TCH	C17-C13-C14	-5.25	94.80	100.09
3	A	601	TCH	C17-C13-C14	-5.08	94.97	100.09
3	B	602	TCH	C14-C8-C9	5.04	116.62	109.71
3	A	602	TCH	C15-C14-C8	5.01	125.33	118.33
3	B	601	TCH	C13-C14-C8	-4.99	108.37	114.74
3	A	602	TCH	C4-C3-C2	-4.94	104.65	110.55
3	A	601	TCH	C4-C3-C2	-4.93	104.66	110.55
3	B	601	TCH	O24-C24-N24	-4.89	113.78	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	TCH	O24-C24-N24	-4.88	113.81	123.01
3	B	602	TCH	C11-C12-C13	4.72	116.09	111.24
3	A	602	TCH	C5-C4-C3	-4.70	105.85	112.76
3	B	602	TCH	O24-C24-N24	-4.66	114.22	123.01
3	A	601	TCH	C6-C5-C4	4.62	116.51	111.19
3	A	601	TCH	C14-C8-C7	4.62	117.93	111.81
3	B	601	TCH	C14-C8-C7	4.57	117.86	111.81
3	B	602	TCH	C9-C8-C7	-4.54	106.44	111.88
3	B	602	TCH	C13-C17-C20	4.52	124.89	119.50
3	A	601	TCH	C14-C8-C9	4.43	115.80	109.71
3	A	602	TCH	O24-C24-N24	-4.17	115.15	123.01
3	B	601	TCH	C18-C13-C14	-4.12	104.76	111.21
3	A	601	TCH	C13-C14-C8	-4.05	109.56	114.74
3	A	601	TCH	C14-C13-C12	-3.96	103.71	107.40
3	A	601	TCH	C18-C13-C14	-3.96	105.02	111.21
3	B	602	TCH	C4-C5-C10	-3.93	108.48	112.66
3	B	602	TCH	C10-C9-C8	3.93	116.04	111.82
3	A	602	TCH	C14-C8-C9	3.93	115.10	109.71
3	B	601	TCH	C5-C4-C3	-3.92	107.00	112.76
3	B	601	TCH	C26-C25-N24	3.78	122.37	111.30
3	A	602	TCH	C18-C13-C14	-3.77	105.31	111.21
3	B	602	TCH	C16-C15-C14	-3.68	97.85	105.13
3	A	602	TCH	C13-C14-C8	-3.63	110.10	114.74
3	B	602	TCH	C23-C22-C20	3.63	121.15	114.52
3	B	602	TCH	C13-C14-C8	-3.60	110.14	114.74
3	A	602	TCH	C21-C20-C17	-3.52	107.53	112.92
3	A	601	TCH	C26-C25-N24	3.48	121.49	111.30
3	B	601	TCH	C14-C8-C9	3.47	114.47	109.71
3	A	602	TCH	C16-C15-C14	-3.44	98.32	105.13
3	B	601	TCH	C23-C22-C20	3.36	120.65	114.52
3	B	602	TCH	C26-C25-N24	3.31	120.98	111.30
3	B	602	TCH	C18-C13-C14	-3.29	106.07	111.21
3	A	602	TCH	C26-C25-N24	3.24	120.77	111.30
3	B	602	TCH	O1S-S26-C26	-3.21	103.05	106.92
3	B	602	TCH	C4-C3-C2	-3.17	106.76	110.55
3	A	601	TCH	C23-C22-C20	3.16	120.30	114.52
3	B	602	TCH	C6-C7-C8	3.15	114.84	111.48
3	A	601	TCH	C5-C4-C3	-3.07	108.25	112.76
3	A	601	TCH	O1S-S26-C26	-3.07	103.22	106.92
3	A	601	TCH	O3-C3-C2	3.05	117.94	110.16
3	B	601	TCH	O3-C3-C2	3.03	117.88	110.16
3	A	601	TCH	C16-C15-C14	-3.03	99.13	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	TCH	C15-C16-C17	2.99	111.05	105.13
3	B	601	TCH	C15-C16-C17	2.96	110.99	105.13
3	B	601	TCH	C16-C15-C14	-2.95	99.28	105.13
3	A	601	TCH	C5-C6-C7	-2.95	111.21	114.46
3	B	601	TCH	C21-C20-C17	-2.94	108.42	112.92
3	A	602	TCH	O3-C3-C2	2.90	117.54	110.16
3	A	602	TCH	C6-C5-C10	-2.89	109.59	112.66
3	A	601	TCH	C19-C10-C5	2.84	115.18	110.36
3	A	602	TCH	C23-C22-C20	2.78	119.59	114.52
3	A	601	TCH	C22-C20-C17	2.73	115.93	110.28
3	A	602	TCH	C1-C10-C9	-2.68	107.14	111.35
3	B	602	TCH	C5-C4-C3	-2.64	108.88	112.76
3	B	602	TCH	C19-C10-C5	2.64	114.84	110.36
3	B	601	TCH	C6-C5-C10	-2.64	109.86	112.66
3	A	602	TCH	C19-C10-C5	2.63	114.83	110.36
3	A	602	TCH	C15-C16-C17	2.59	110.26	105.13
3	B	601	TCH	O1S-S26-C26	-2.59	103.80	106.92
3	A	601	TCH	C4-C5-C10	-2.58	109.92	112.66
3	B	601	TCH	C19-C10-C5	2.55	114.69	110.36
3	A	602	TCH	C14-C8-C7	2.49	115.10	111.81
3	B	602	TCH	O3-C3-C2	2.48	116.47	110.16
2	B	600	NAG	C1-O5-C5	2.47	115.53	112.19
3	A	601	TCH	C21-C20-C17	-2.46	109.15	112.92
3	B	602	TCH	C15-C16-C17	2.45	109.99	105.13
3	A	601	TCH	O7-C7-C6	2.39	115.88	109.94
3	A	601	TCH	C19-C10-C9	-2.38	107.90	111.18
3	A	602	TCH	O1S-S26-C26	-2.38	104.05	106.92
3	B	602	TCH	C9-C10-C5	-2.36	105.27	108.58
3	A	602	TCH	C6-C7-C8	2.35	113.99	111.48
3	B	602	TCH	C16-C17-C20	2.32	115.74	112.15
3	A	601	TCH	C1-C2-C3	-2.30	107.52	110.47
2	B	600	NAG	C8-C7-N2	-2.27	112.26	116.10
3	B	602	TCH	O7-C7-C6	2.27	115.57	109.94
2	A	600	NAG	C8-C7-N2	-2.20	112.38	116.10
3	B	601	TCH	C6-C7-C8	2.18	113.81	111.48
3	A	602	TCH	C14-C13-C12	-2.18	105.38	107.40
3	B	601	TCH	O24-C24-C23	-2.17	118.05	122.02
3	B	601	TCH	C22-C20-C17	2.11	114.65	110.28
3	B	602	TCH	O24-C24-C23	-2.09	118.19	122.02
2	A	600	NAG	C1-O5-C5	2.05	114.97	112.19
3	B	601	TCH	C1-C2-C3	-2.04	107.85	110.47
3	A	601	TCH	O24-C24-C23	-2.02	118.32	122.02

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	TCH	C3
3	A	601	TCH	C20
3	A	601	TCH	C5
3	A	601	TCH	C9
3	A	602	TCH	C3
3	A	602	TCH	C20
3	A	602	TCH	C5
3	A	602	TCH	C9
3	B	601	TCH	C3
3	B	601	TCH	C20
3	B	601	TCH	C5
3	B	601	TCH	C9
3	B	602	TCH	C3
3	B	602	TCH	C20
3	B	602	TCH	C5
3	B	602	TCH	C9

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	TCH	C13-C17-C20-C22
3	A	601	TCH	C16-C17-C20-C22
3	A	601	TCH	C23-C24-N24-C25
3	A	601	TCH	N24-C25-C26-S26
3	A	602	TCH	C25-C26-S26-O1S
3	A	602	TCH	C25-C26-S26-O2S
3	B	601	TCH	C16-C17-C20-C22
3	B	601	TCH	N24-C25-C26-S26
3	B	602	TCH	C13-C17-C20-C21
3	B	602	TCH	O24-C24-N24-C25
3	B	602	TCH	C26-C25-N24-C24
3	B	602	TCH	N24-C25-C26-S26
3	B	601	TCH	O24-C24-N24-C25
3	B	601	TCH	C16-C17-C20-C21
3	B	602	TCH	C21-C20-C22-C23
3	A	601	TCH	C13-C17-C20-C21
3	B	602	TCH	C16-C17-C20-C22
3	B	602	TCH	C13-C17-C20-C22
3	B	602	TCH	C16-C17-C20-C21
3	A	602	TCH	C13-C17-C20-C22
3	B	601	TCH	C13-C17-C20-C22
3	A	601	TCH	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	601	TCH	C21-C20-C22-C23
3	A	601	TCH	C16-C17-C20-C21
3	A	602	TCH	C16-C17-C20-C22
3	A	602	TCH	C13-C17-C20-C21
3	B	602	TCH	C17-C20-C22-C23
3	B	601	TCH	C22-C23-C24-O24
3	A	602	TCH	C16-C17-C20-C21
3	B	601	TCH	C22-C23-C24-N24
3	B	601	TCH	C21-C20-C22-C23
3	B	602	TCH	C23-C24-N24-C25
3	B	601	TCH	C17-C20-C22-C23
3	A	602	TCH	C25-C26-S26-O3S
3	B	602	TCH	C20-C22-C23-C24
2	A	600	NAG	C1-C2-N2-C7
2	A	600	NAG	C3-C2-N2-C7
3	B	601	TCH	C13-C17-C20-C21
3	A	602	TCH	C20-C22-C23-C24
3	A	601	TCH	O24-C24-N24-C25
2	B	600	NAG	C1-C2-N2-C7
2	B	600	NAG	C3-C2-N2-C7

There are no ring outliers.

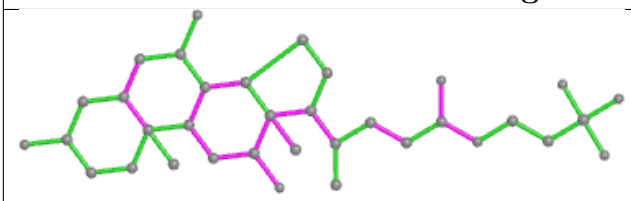
6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	NAG	1	0
2	A	600	NAG	2	0
3	A	601	TCH	1	0
3	B	601	TCH	7	0
3	A	602	TCH	8	0
3	B	602	TCH	4	0

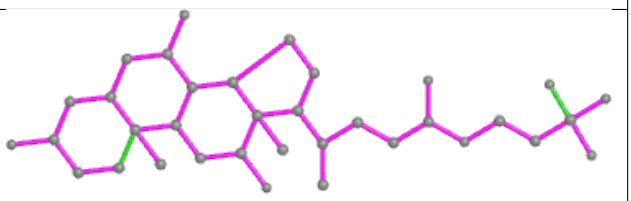
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

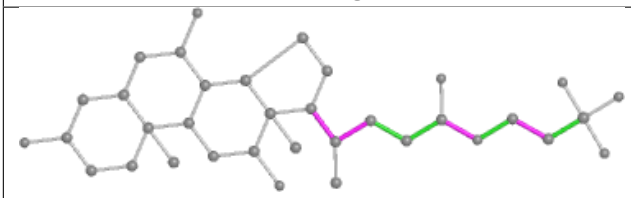
Ligand TCH A 601



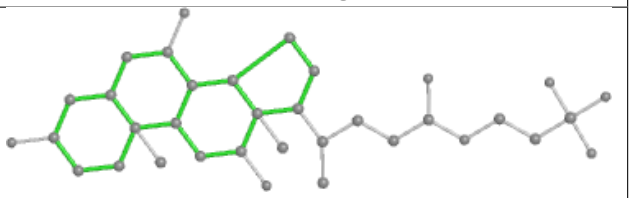
Bond lengths



Bond angles

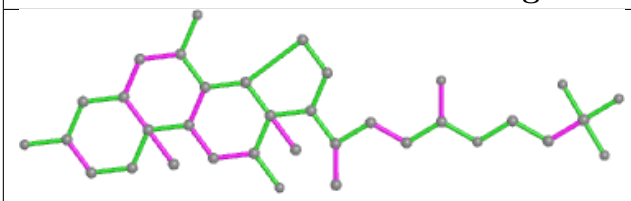


Torsions

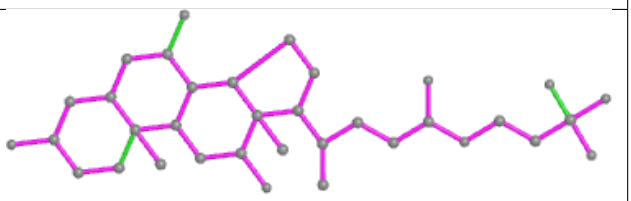


Rings

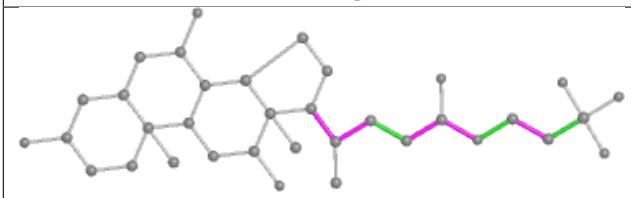
Ligand TCH B 601



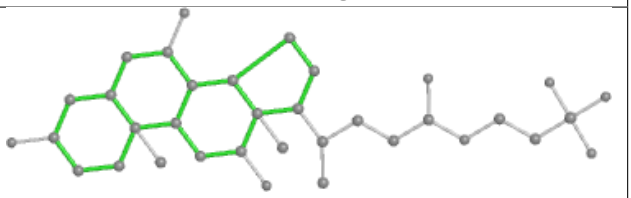
Bond lengths



Bond angles

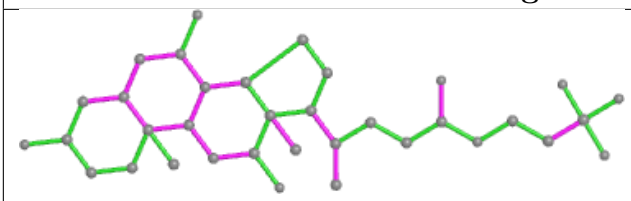


Torsions

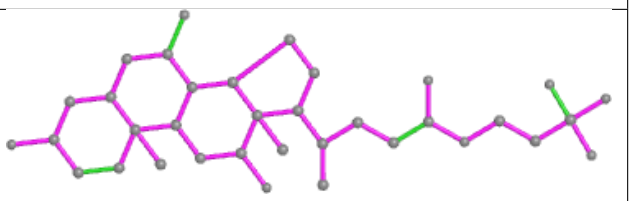


Rings

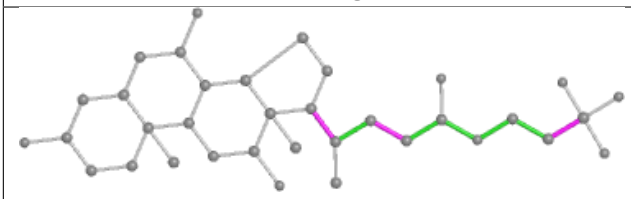
Ligand TCH A 602



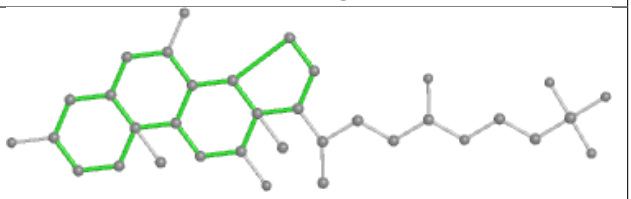
Bond lengths



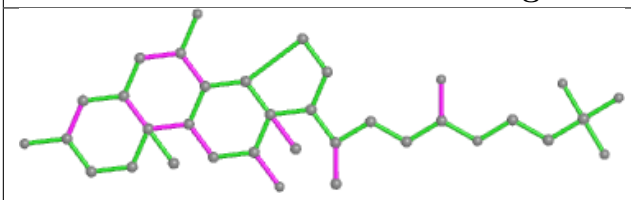
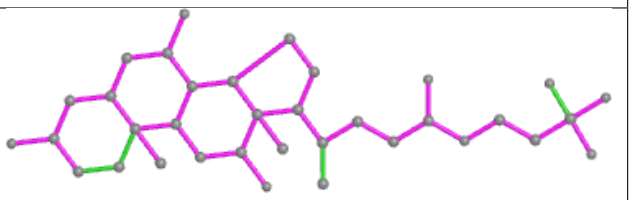
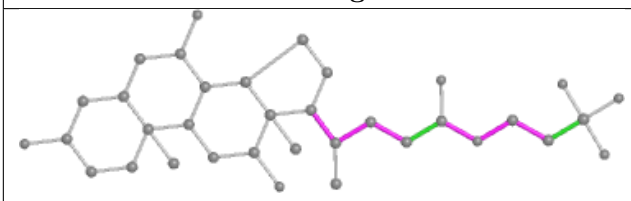
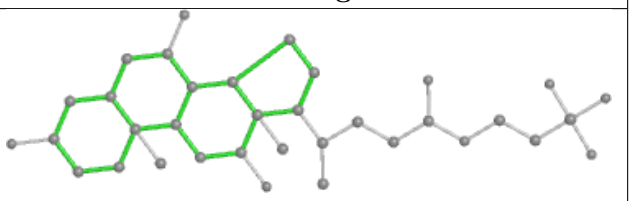
Bond angles



Torsions



Rings

Ligand TCH B 602	
 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.