



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:50 AM GMT

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 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/ValidationPDFNotes.html>

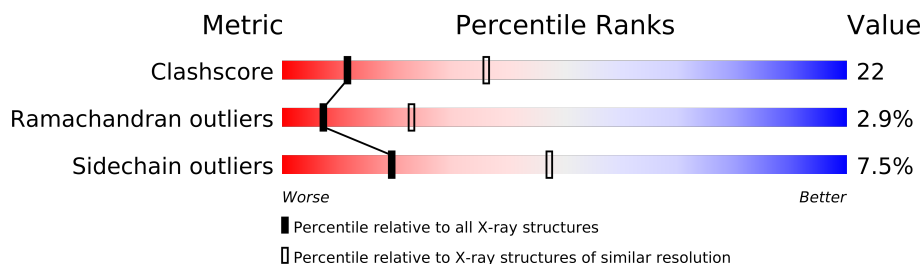
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	532	
1	B	532	

2 Entry composition (i)

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

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.

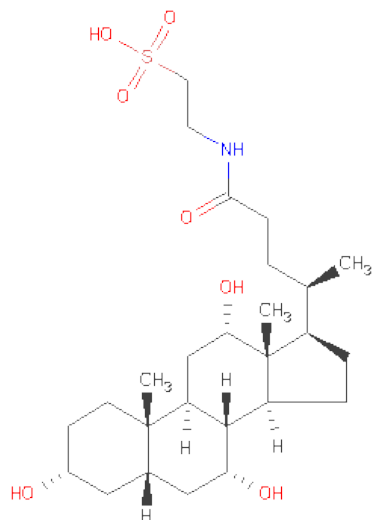
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			
1	B	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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



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

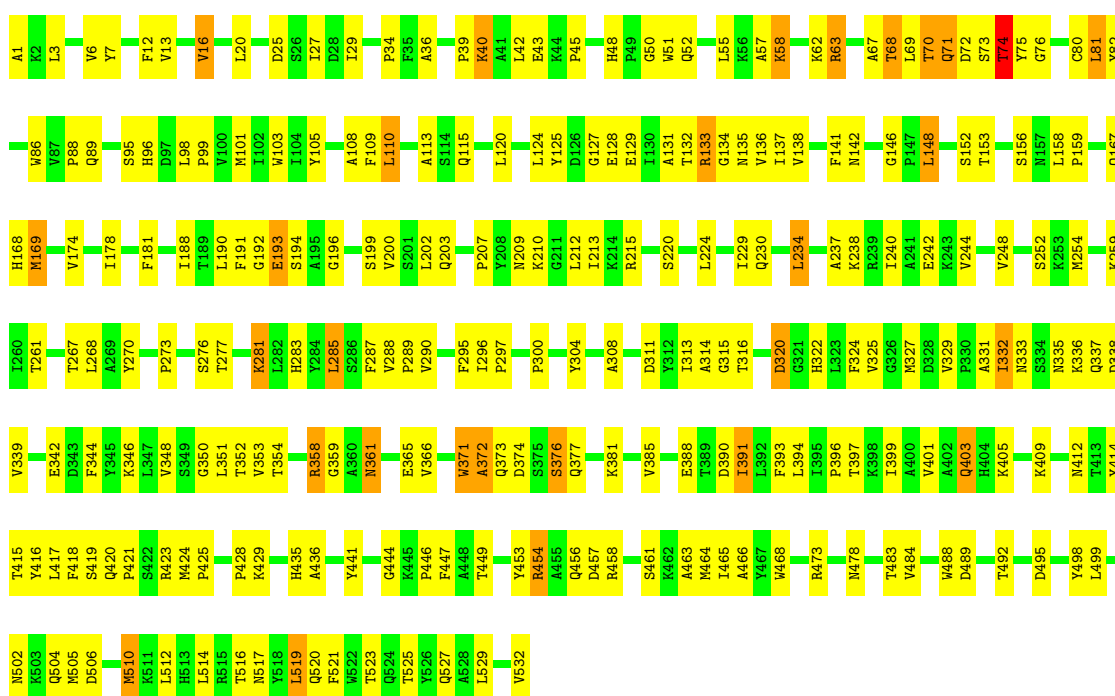
3 Residue-property plots

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

Note EDS was not executed.

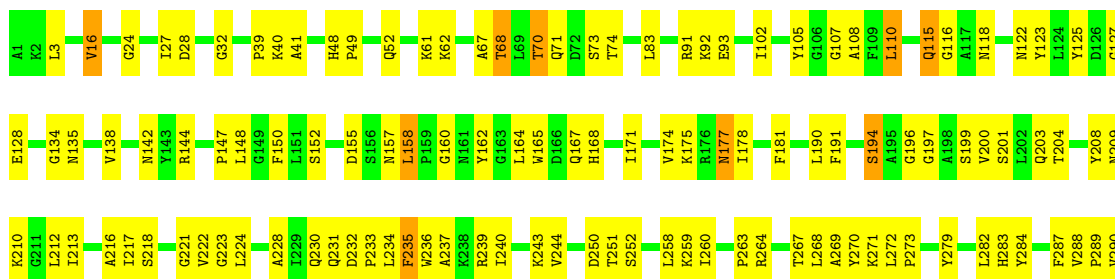
• Molecule 1: BILE-SALT ACTIVATED LIPASE

Chain A:



• Molecule 1: BILE-SALT ACTIVATED LIPASE

Chain B:



T525	Q440	E385	T291
Y526	Y441	E369	D294
Q527	Y442	E370	F295
P530	G443	W371	T296
T531	G444	A372	P297
V532	K445	Q373	D298
	P446	Q374	D299
	F447	Q375	P300
	A448	Q377	V301
	T449		N302
	P450	R380	L303
L451	L451	K381	Y304
G452	G452	K382	
Y453	R454	T383	A308
A455	A455	K384	D309
Q456	Q456	V385	V310
D457	D457	D386	
T458	T458	L387	T313
T459	T459	E388	A314
S461	S461	T389	
K462	K462	D390	D318
		T391	M319
		L392	D320
I465	I465	F393	G321
		L394	H322
W468	W468	T395	
T469	T469	F396	V325
		T397	
R473	R473	K398	P330
T474	T474	T399	A331
		A400	I332
T483	T483	V401	N333
			S334
D489	D489	H404	N335
P490	P490		K336
E494	E494	A408	Q337
D495	D495	K409	D338
A496	A496	M412	V339
N497	N497	T413	T340
Y498	Y498	Y414	F341
		T415	E342
K503	K503	Y416	D343
Q504	Q504	L417	
			K346
S507	S507	R423	G350
		M424	L351
M510	M510		T352
L511	L511	Y427	
L512	L512	P428	K355
H513	H513	K429	G356
L514	L514	W430	L357
R515	R515	M431	R358
			G359
L519	L519	H435	A360
Q520	Q520	A436	N361
F521	F521	D437	A362
W522	W522	D438	T363
		F439	V363

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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: NAG, TCH

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8498	0	8300	369	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (369) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:67:ALA:HA	1:B:73:SER:HA	1.37	1.04
1:B:115:GLN:HE21	1:B:115:GLN:H	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:418:PHE:HE1	1:A:464:MET:SD	2.02	0.81
1:A:342:GLU:HG2	1:A:346:LYS:HE3	1.60	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:B:295:PHE:O	1:B:297:PRO:HD3	1.85	0.75
1:A:99:PRO:HB2	1:A:136:VAL:HG23	1.67	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:H	1:A:148:LEU:HD12	1.55	0.72
1:B:357:LEU:HA	1:B:360:ALA:HB3	1.71	0.72
1:A:372:ALA:HB1	1:A:376:SER:HB2	1.73	0.71
1:A:196:GLY:O	1:A:200:VAL:HG23	1.89	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
3:B:602:TCH:H7	3:B:602:TCH:H19	1.71	0.70
1:B:288:VAL:HB	1:B:289:PRO:HD2	1.72	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:418:PHE:CE1	1:A:464:MET:SD	2.85	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:NE2	1:B:115:GLN:H	1.89	0.66
1:B:273:PRO:HG2	1:B:284:TYR:CD2	2.30	0.66
1:B:230:GLN:HB3	1:B:290:VAL:HG12	1.77	0.66
1:B:115:GLN:N	1:B:115:GLN:HE21	1.89	0.65
1:A:396:PRO:HG3	3:A:602:TCH:H16	1.79	0.65
1:A:338:ASP:HA	1:A:381:LYS:HZ3	1.61	0.65
1:B:338:ASP:HB2	1:B:377:GLN:NE2	2.12	0.65
1:A:68:THR:HB	1:A:71:GLN:OE1	1.96	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:HB3	1:A:409:LYS:NZ	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:333:ASN:OD1	1:A:336:LYS:HG3	2.00	0.61
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: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:391:ILE:CB	3:A:602:TCH:H21	2.32	0.60
1:A:230:GLN:HB3	1:A:290:VAL:HG12	1.83	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:264:ARG:HD2	1:B:264:ARG:H	1.66	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:39:PRO:HB2	1:B:144:ARG:NH1	2.18	0.59
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:391:ILE:CG2	3:A:602:TCH:H21	2.33	0.57
1:A:108:ALA:HB3	1:A:110:LEU:CD2	2.34	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:B:218:SER:O	1:B:314:ALA:HA	2.05	0.57
1:A:316:THR:O	1:A:417:LEU:HD12	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:B:444:GLY:CA	1:B:465:ILE:HD11	2.35	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: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:372:ALA:HB1	1:A:376:SER:CB	2.36	0.55
1:A:73:SER:HB2	1:A:268:LEU:HG	1.88	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:B:135:ASN:HB3	1:B:473:ARG:NH2	2.23	0.54
1:A:344:PHE:O	1:A:348:VAL:HG23	2.07	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:338:ASP:HB2	1:B:377:GLN:HE22	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:291:ILE:HG23	1:B:296:ILE:HG22	1.89	0.54
3:B:601:TCH:H18B	3:B:601:TCH:H22	1.89	0.53
1:A:63:ARG:HE	1:A:113:ALA:HB2	1.73	0.53
1:A:358:ARG:CG	1:A:529:LEU:HD13	2.38	0.53
1:B:190:LEU:HB2	1:B:213:ILE:HD12	1.90	0.53
1:A:153:THR:O	1:A:234:LEU:HD22	2.09	0.53
1:A:108:ALA:HB3	1:A:110:LEU:HD22	1.90	0.53
1:B:222:VAL:HG21	1:B:400:ALA:HB1	1.90	0.53
1:A:229:ILE:HD13	1:A:289:PRO:HB2	1.90	0.53
1:A:42:LEU:HB3	1:A:158:LEU:HD11	1.91	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:272:LEU:HD23	1:B:273:PRO:HD2	1.90	0.52
1:B:174:VAL:O	1:B:178:ILE:HB	2.09	0.52
1:B:449:THR:O	1:B:449:THR:HG23	2.08	0.52
1:B:522:TRP:O	1:B:527:GLN:HG2	2.09	0.52
1:B:449:THR:CG2	3:B:601:TCH:H15	2.39	0.52
1:A:495:ASP:HB3	1:A:512:LEU:CD2	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:B:230:GLN:NE2	1:B:232:ASP:H	2.08	0.51
1:A:234:LEU:O	1:A:234:LEU:HD12	2.11	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:B:118:ASN:HB3	1:B:123:TYR:CD1	2.46	0.50
1:A:48:HIS:HD2	1:A:50:GLY:H	1.57	0.50
1:B:458:ARG:O	1:B:462:LYS:HB2	2.10	0.50
1:B:158:LEU:HD12	1:B:162:TYR:OH	2.11	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:B:199:SER:O	1:B:203:GLN:HG2	2.10	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
1:B:325:VAL:HG11	1:B:385:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:405:LYS:NZ	1:A:492:THR:HA	2.27	0.50
1:A:366:VAL:HG11	1:A:521:PHE:CZ	2.46	0.50
1:A:168:HIS:CD2	1:A:209:ASN:OD1	2.65	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:B:446:PRO:HG3	1:B:453:TYR:CD2	2.47	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:495:ASP:HB3	1:B:512:LEU:CD2	2.40	0.49
1:A:3:LEU:HD21	1:A:181:PHE:HA	1.95	0.49
1:B:449:THR:OG1	3:B:601:TCH:H15	2.13	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:A:281:LYS:H	1:A:281:LYS:HD3	1.78	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:B:150:PHE:HE1	1:B:164:LEU:CD2	2.26	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: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:B:298:ASP:H	1:B:303:LEU:HD21	1.79	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: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:380:ARG:HA	1:B:383:THR:OG1	2.15	0.47
1:A:108:ALA:HB1	1:A:285:LEU:HD21	1.97	0.47
1:B:135:ASN:O	1:B:473:ARG:NH2	2.48	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:152:SER:HB2	1:B:160:GLY:HA3	1.95	0.47
1:A:81:LEU:HD23	1:A:81:LEU:N	2.30	0.46
1:A:339:VAL:H	1:A:381:LYS:HZ1	1.63	0.46
1:B:224:LEU:HD21	1:B:304:TYR:HE1	1.80	0.46
1:A:86:TRP:O	1:A:137:ILE:HG23	2.16	0.46
1:B:92:LYS:HE2	1:B:93:GLU:HG2	1.96	0.46
1:A:68:THR:HG22	1:A:69:LEU:H	1.80	0.46
1:A:13:VAL:CG1	1:A:57:ALA:HB2	2.46	0.46
1:A:339:VAL:H	1:A:381:LYS:NZ	2.14	0.46
1:A:314:ALA:O	1:A:415:THR:HA	2.16	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:B:449:THR:HG21	3:B:601:TCH:HO7	1.81	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:A:62:LYS:HA	1:A:62:LYS:HD2	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:418:PHE:CE2	1:A:420:GLN:HB3	2.51	0.46
1:A:42:LEU:HB2	1:A:259:LYS:HG2	1.98	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:424:MET:HG2	1:B:427:TYR:CE1	2.51	0.45
1:B:369:GLU:N	1:B:370:PRO:HD2	2.32	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
3:B:601:TCH:H22	3:B:601:TCH:C18	2.46	0.45
1:B:102:ILE:HD11	1:B:174:VAL:HG11	1.98	0.45
1:A:517:ASN:O	1:A:520:GLN:HB3	2.17	0.45
1:A:361:ASN:OD1	1:A:361:ASN:N	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232:ASP:N	1:B:233:PRO:HD3	2.32	0.45
1:A:188:ILE:HD12	1:A:212:LEU:O	2.17	0.45
1:B:240:ILE:O	1:B:244:VAL:HG22	2.17	0.45
1:B:497:ASN:HA	1:B:512:LEU:HD23	1.98	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:498:TYR:CE1	1:B:511:LYS:HB2	2.52	0.44
1:A:39:PRO:HD3	1:A:81:LEU:HG	1.99	0.44
1:B:177:ASN:ND2	1:B:177:ASN:N	2.65	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:A:13:VAL:HG13	1:A:55:LEU:HD22	1.98	0.44
1:B:314:ALA:O	1:B:415:THR:HA	2.17	0.44
1:B:167:GLN:O	1:B:171:ILE:HG13	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:B:325:VAL:CB	1:B:388:GLU:HG3	2.35	0.44
1:A:488:TRP:CE3	1:A:499:LEU:HD22	2.53	0.44
1:A:95:SER:HB3	1:A:98:LEU:HD13	2.00	0.44
1:B:191:PHE:CB	1:B:217:ILE:HB	2.47	0.44
1:A:238:LYS:HA	1:A:254:MET:CE	2.47	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:224:LEU:HD23	1:A:300:PRO:HB2	2.00	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:N	1:B:279:TYR:CD1	2.85	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:A:101:MET:HB3	1:A:191:PHE:CE1	2.53	0.44
1:A:7:TYR:HB2	1:A:12:PHE:CE1	2.53	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:340:THR:O	1:B:343:ASP:HB2	2.19	0.43
1:B:62:LYS:HD3	1:B:62:LYS:HA	1.80	0.43
1:B:361:ASN:O	1:B:365:GLU:HG3	2.19	0.43
1:B:318:ASP:HA	1:B:417:LEU:HD11	2.00	0.43
1:B:497:ASN:HB3	1:B:512:LEU:HD23	2.00	0.43
1:B:208:TYR:HE2	1:B:294:ASP:HB2	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:GLY:HA2	1:A:529:LEU:HD12	2.00	0.43
1:A:371:TRP:N	1:A:371:TRP:CD2	2.86	0.43
1:A:1:ALA:HB3	1:A:89:GLN:HB3	1.99	0.43
1:B:332:ILE:H	1:B:332:ILE:HD13	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:337:GLN:CG	1:B:451:LEU:HD21	2.48	0.43
1:A:40:LYS:H	1:A:40:LYS:CD	2.32	0.43
1:B:108:ALA:HB3	1:B:110:LEU:HD23	2.00	0.43
1:B:451:LEU:HA	1:B:451:LEU:HD22	1.74	0.43
1:B:243:LYS:HE2	1:B:269:ALA:HA	2.00	0.43
1:A:454:ARG:N	1:A:454:ARG:HD3	2.34	0.43
1:B:157:ASN:HD22	1:B:252:SER:HA	1.84	0.43
1:A:283:HIS:HE1	1:A:350:GLY:O	2.02	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: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:B:190:LEU:HD22	1:B:213:ILE:HD11	2.01	0.42
1:A:13:VAL:HG22	1:A:51:TRP:HZ2	1.83	0.42
1:B:73:SER:HB2	1:B:268:LEU:HG	2.02	0.42
1:A:358:ARG:HG3	1:A:529:LEU:HD13	2.00	0.42
1:A:352:THR:O	1:A:354:THR:N	2.52	0.42
1:A:174:VAL:O	1:A:178:ILE:HB	2.19	0.42
1:A:420:GLN:HA	1:A:421:PRO:HD2	1.89	0.42
1:A:207:PRO:HD2	1:A:295:PHE:O	2.20	0.42
1:B:243:LYS:HB3	1:B:243:LYS:HE3	1.90	0.42
1:A:58:LYS:HD3	1:A:58:LYS:C	2.39	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: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:A:215:ARG:HD3	1:A:311:ASP:HB2	2.02	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:336:LYS:HD3	1:B:451:LEU:CD2	2.42	0.41
1:A:193:GLU:O	1:A:196:GLY:N	2.52	0.41
1:B:338:ASP:HB2	1:B:377:GLN:OE1	2.19	0.41
1:A:320:ASP:OD1	1:A:435:HIS:HA	2.20	0.41
3:A:601:TCH:H11A	3:A:601:TCH:H1A	1.81	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:A:190:LEU:HD23	1:A:213:ILE:HG12	2.02	0.41
1:A:152:SER:O	1:A:237:ALA:HB2	2.21	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:352:THR:HG22	1:B:526:TYR:CE2	2.56	0.41
1:B:105:TYR:HE2	1:B:142:ASN:HA	1.86	0.41
1:B:489:ASP:HA	1:B:490:PRO:HD3	1.91	0.41
1:A:240:ILE:O	1:A:244:VAL:HG22	2.20	0.41
1:A:441:TYR:HE2	1:A:457:ASP:HA	1.85	0.41
1:A:390:ASP:HA	1:A:394:LEU:HB3	2.01	0.41
1:B:115:GLN:HG2	1:B:116:GLY:N	2.36	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: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:NZ	1:A:429:LYS:HB2	2.36	0.40
1:A:88:PRO:HG3	1:A:131:ALA:HB1	2.02	0.40
1:A:20:LEU:HB2	1:A:25:ASP:O	2.21	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:412:ASN:HB2	1:A:414:TYR:HE1	1.87	0.40
3:B:601:TCH:H6A	3:B:601:TCH:H19	1.94	0.40
1:A:401:VAL:HG11	1:A:415:THR:HB	2.04	0.40
1:A:134:GLY:O	1:A:473:ARG:NH2	2.54	0.40
1:B:332:ILE:O	1:B:428:PRO:HG3	2.21	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
1:A:133:ARG:CZ	1:A:447:PHE:CD2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/532 (100%)	451 (85%)	63 (12%)	16 (3%)	7	22
1	B	530/532 (100%)	456 (86%)	59 (11%)	15 (3%)	8	24
All	All	1060/1064 (100%)	907 (86%)	122 (12%)	31 (3%)	7	23

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
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

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Mol	Chain	Res	Type
1	A	68	THR
1	B	513	HIS
1	B	107	GLY
1	B	330	PRO

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	444/444 (100%)	403 (91%)	41 (9%)	13	36
1	B	444/444 (100%)	418 (94%)	26 (6%)	28	62
All	All	888/888 (100%)	821 (92%)	67 (8%)	19	47

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	483	THR
1	B	507	SER
1	B	519	LEU
1	B	530	PRO

Some 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 ⓘ

There are no RNA chains 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

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	A	600	1	12,14,15	0.63	0	15,19,21	0.81	0
3	TCH	A	601	-	38,38,38	2.04	11 (28%)	60,60,60	4.82	36 (60%)
3	TCH	A	602	-	38,38,38	2.17	12 (31%)	60,60,60	4.92	37 (61%)
2	NAG	B	600	1	12,14,15	0.82	1 (8%)	15,19,21	0.88	0
3	TCH	B	601	-	38,38,38	2.04	10 (26%)	60,60,60	4.73	34 (56%)
3	TCH	B	602	-	38,38,38	1.99	10 (26%)	60,60,60	4.72	35 (58%)

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	A	600	1	-	0/6/23/26	0/1/1/1
3	TCH	A	601	-	4/4/13/14	0/16/81/81	0/0/4/4
3	TCH	A	602	-	4/4/13/14	0/16/81/81	0/0/4/4
2	NAG	B	600	1	-	0/6/23/26	0/1/1/1
3	TCH	B	601	-	4/4/13/14	0/16/81/81	0/0/4/4
3	TCH	B	602	-	4/4/13/14	0/16/81/81	0/0/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	TCH	C6-C5	-5.30	1.44	1.53
3	B	602	TCH	C10-C9	-5.23	1.47	1.56
3	A	602	TCH	C6-C5	-5.07	1.45	1.53
3	A	602	TCH	C10-C5	-4.96	1.46	1.55
3	A	601	TCH	C8-C9	4.81	1.63	1.53
3	B	602	TCH	C11-C9	-4.68	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	TCH	C10-C5	-4.37	1.47	1.55
3	A	602	TCH	C6-C7	-4.18	1.45	1.52
3	A	602	TCH	C11-C9	-4.15	1.46	1.53
3	B	601	TCH	C11-C12	4.07	1.60	1.53
3	A	602	TCH	C8-C7	-3.98	1.46	1.53
3	B	601	TCH	C10-C5	-3.86	1.48	1.55
3	B	602	TCH	C18-C13	3.78	1.60	1.54
3	A	601	TCH	C18-C13	3.76	1.60	1.54
3	B	601	TCH	C11-C9	-3.70	1.47	1.53
3	A	601	TCH	C20-C17	3.60	1.61	1.54
3	A	601	TCH	C11-C9	-3.58	1.47	1.53
3	A	601	TCH	O24-C24	3.24	1.30	1.23
3	A	601	TCH	C10-C5	-3.22	1.49	1.55
3	B	602	TCH	C6-C7	3.13	1.58	1.52
3	B	601	TCH	C8-C9	3.11	1.60	1.53
3	B	601	TCH	C6-C7	-3.07	1.47	1.52
3	A	602	TCH	C21-C20	-3.00	1.45	1.53
3	A	602	TCH	O24-C24	2.96	1.29	1.23
3	A	602	TCH	C10-C9	-2.93	1.51	1.56
3	A	601	TCH	C13-C17	2.90	1.60	1.55
3	B	602	TCH	C4-C3	2.90	1.57	1.51
3	B	602	TCH	C8-C7	2.89	1.58	1.53
3	A	601	TCH	C24-N24	2.87	1.40	1.33
3	B	602	TCH	O24-C24	2.69	1.29	1.23
3	A	601	TCH	C8-C14	2.62	1.59	1.53
3	B	601	TCH	O24-C24	2.59	1.29	1.23
3	A	602	TCH	C18-C13	2.58	1.58	1.54
3	B	601	TCH	C18-C13	2.57	1.58	1.54
3	B	602	TCH	O12-C12	2.52	1.48	1.43
3	A	601	TCH	C6-C5	-2.42	1.49	1.53
3	A	602	TCH	C8-C14	-2.42	1.48	1.53
2	B	600	NAG	C2-N2	2.38	1.49	1.46
3	A	602	TCH	C8-C9	2.30	1.58	1.53
3	B	601	TCH	C22-C23	2.26	1.60	1.52
3	A	602	TCH	C11-C12	2.10	1.57	1.53
3	B	601	TCH	C26-S26	2.10	1.80	1.77
3	B	602	TCH	C21-C20	-2.05	1.47	1.53
3	A	601	TCH	C13-C12	2.05	1.57	1.54

All (142) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	TCH	O2S-S26-C26	16.11	120.61	106.81
3	A	602	TCH	O2S-S26-C26	16.07	120.58	106.81
3	B	602	TCH	O2S-S26-C26	15.41	120.02	106.81
3	A	602	TCH	C15-C14-C13	14.53	118.12	103.58
3	B	601	TCH	O2S-S26-C26	14.04	118.84	106.81
3	B	601	TCH	C15-C14-C13	14.01	117.61	103.58
3	B	602	TCH	C11-C9-C8	13.51	130.24	110.81
3	A	601	TCH	C15-C14-C13	13.47	117.06	103.58
3	B	602	TCH	C15-C14-C13	12.73	116.33	103.58
3	A	601	TCH	C11-C9-C8	12.05	128.13	110.81
3	A	602	TCH	C11-C9-C8	11.86	127.86	110.81
3	B	601	TCH	C11-C9-C8	11.74	127.70	110.81
3	B	602	TCH	C9-C11-C12	-10.90	100.12	114.35
3	A	601	TCH	C9-C11-C12	-10.52	100.62	114.35
3	A	602	TCH	C9-C11-C12	-9.73	101.65	114.35
3	A	602	TCH	C5-C6-C7	-8.67	105.22	114.46
3	B	601	TCH	C9-C11-C12	-8.38	103.42	114.35
3	A	602	TCH	C10-C9-C8	7.91	120.31	111.90
3	B	601	TCH	C11-C12-C13	7.87	119.28	111.21
3	B	601	TCH	C10-C9-C8	7.73	120.12	111.90
3	B	602	TCH	O12-C12-C11	7.65	124.38	108.99
3	A	601	TCH	C18-C13-C12	7.62	116.68	109.08
3	B	601	TCH	O12-C12-C11	7.35	123.78	108.99
3	A	602	TCH	O12-C12-C11	7.23	123.55	108.99
3	A	602	TCH	C18-C13-C12	6.98	116.05	109.08
3	A	601	TCH	C10-C9-C8	6.87	119.20	111.90
3	A	602	TCH	C6-C5-C4	6.87	119.30	111.14
3	A	601	TCH	O12-C12-C11	6.66	122.39	108.99
3	A	601	TCH	C13-C17-C20	6.66	127.52	119.51
3	B	601	TCH	O3-C3-C4	6.64	123.10	109.87
3	B	602	TCH	C15-C14-C8	6.47	127.49	118.30
3	A	602	TCH	O3-C3-C4	6.44	122.72	109.87
3	A	601	TCH	O3-C3-C4	6.43	122.68	109.87
3	B	601	TCH	C5-C6-C7	-6.40	107.64	114.46
3	A	601	TCH	C11-C12-C13	6.22	117.59	111.21
3	B	601	TCH	C18-C13-C12	6.21	115.28	109.08
3	B	602	TCH	C18-C13-C12	6.20	115.27	109.08
3	B	601	TCH	C16-C17-C13	6.19	109.77	103.58
3	A	602	TCH	C11-C12-C13	6.04	117.41	111.21
3	A	601	TCH	C15-C14-C8	6.03	126.86	118.30
3	B	602	TCH	O3-C3-C4	5.97	121.76	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TCH	C17-C13-C14	-5.77	94.17	100.07
3	A	602	TCH	C13-C17-C20	5.71	126.38	119.51
3	B	601	TCH	C6-C5-C4	5.70	117.91	111.14
3	B	601	TCH	C13-C14-C8	-5.68	108.37	114.81
3	B	602	TCH	C14-C8-C7	5.64	118.78	111.81
3	A	602	TCH	C16-C17-C13	5.55	109.13	103.58
3	A	602	TCH	C17-C13-C14	-5.52	94.43	100.07
3	B	601	TCH	C15-C14-C8	5.45	126.04	118.30
3	B	601	TCH	C13-C17-C20	5.35	125.94	119.51
3	B	602	TCH	C6-C5-C4	5.32	117.46	111.14
3	A	601	TCH	C16-C17-C13	5.30	108.89	103.58
3	B	602	TCH	C14-C8-C9	5.24	116.62	109.61
3	B	601	TCH	C17-C13-C14	-5.16	94.80	100.07
3	B	602	TCH	C16-C17-C13	5.15	108.73	103.58
3	A	601	TCH	C17-C13-C14	-4.99	94.97	100.07
3	A	602	TCH	C15-C14-C8	4.95	125.33	118.30
3	A	601	TCH	C14-C8-C7	4.95	117.93	111.81
3	B	602	TCH	C9-C8-C7	-4.95	106.44	111.97
3	B	601	TCH	C4-C3-C2	-4.94	104.22	110.54
3	B	601	TCH	C14-C8-C7	4.90	117.86	111.81
3	A	602	TCH	C5-C4-C3	-4.84	105.85	112.95
3	B	602	TCH	C11-C12-C13	4.76	116.09	111.21
3	A	601	TCH	C13-C14-C8	-4.63	109.56	114.81
3	A	601	TCH	C14-C8-C9	4.62	115.80	109.61
3	B	601	TCH	O24-C24-N24	-4.62	113.78	122.94
3	A	602	TCH	C4-C3-C2	-4.60	104.65	110.54
3	A	601	TCH	O24-C24-N24	-4.60	113.81	122.94
3	A	601	TCH	C4-C3-C2	-4.60	104.66	110.54
3	A	601	TCH	C6-C5-C4	4.52	116.51	111.14
3	B	602	TCH	C13-C17-C20	4.47	124.89	119.51
3	B	602	TCH	O24-C24-N24	-4.40	114.22	122.94
3	B	602	TCH	O1S-S26-C26	-4.39	103.05	106.81
3	B	602	TCH	C23-C22-C20	4.23	121.15	114.46
3	A	601	TCH	O1S-S26-C26	-4.19	103.22	106.81
3	A	602	TCH	C13-C14-C8	-4.15	110.10	114.81
3	B	602	TCH	C13-C14-C8	-4.12	110.14	114.81
3	A	602	TCH	C14-C8-C9	4.10	115.10	109.61
3	B	601	TCH	C18-C13-C14	-4.07	104.76	111.22
3	B	601	TCH	C5-C4-C3	-4.06	107.00	112.95
3	A	601	TCH	C14-C13-C12	-3.98	103.71	107.40
3	A	602	TCH	O24-C24-N24	-3.93	115.15	122.94
3	B	601	TCH	C23-C22-C20	3.91	120.65	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	TCH	C18-C13-C14	-3.91	105.02	111.22
3	B	602	TCH	C10-C9-C8	3.89	116.04	111.90
3	B	602	TCH	C4-C5-C10	-3.87	108.48	112.67
3	A	602	TCH	C18-C13-C14	-3.72	105.31	111.22
3	A	601	TCH	C23-C22-C20	3.69	120.30	114.46
3	B	602	TCH	C25-C26-S26	-3.66	104.10	113.66
3	A	602	TCH	C25-C26-S26	-3.65	104.12	113.66
3	B	601	TCH	C14-C8-C9	3.63	114.47	109.61
3	B	602	TCH	C16-C15-C14	-3.59	97.85	105.14
3	B	601	TCH	C26-C25-N24	3.58	122.37	111.21
3	A	601	TCH	C25-C26-S26	-3.58	104.30	113.66
3	B	601	TCH	O1S-S26-C26	-3.51	103.80	106.81
3	A	602	TCH	C16-C15-C14	-3.36	98.32	105.14
3	A	601	TCH	C26-C25-N24	3.30	121.49	111.21
3	B	602	TCH	C18-C13-C14	-3.24	106.07	111.22
3	A	602	TCH	C23-C22-C20	3.24	119.59	114.46
3	A	602	TCH	O1S-S26-C26	-3.22	104.05	106.81
3	A	601	TCH	C5-C4-C3	-3.20	108.25	112.95
3	B	602	TCH	C6-C7-C8	3.15	114.84	111.51
3	B	602	TCH	C26-C25-N24	3.14	120.98	111.21
3	A	602	TCH	C21-C20-C17	-3.10	107.53	112.96
3	A	602	TCH	C26-C25-N24	3.07	120.77	111.21
3	A	601	TCH	C5-C6-C7	-3.05	111.21	114.46
3	A	601	TCH	C16-C15-C14	-2.96	99.13	105.14
3	B	602	TCH	C4-C3-C2	-2.95	106.76	110.54
3	A	601	TCH	C15-C16-C17	2.91	111.05	105.14
3	B	601	TCH	C16-C15-C14	-2.89	99.28	105.14
3	B	601	TCH	C15-C16-C17	2.88	110.99	105.14
3	A	602	TCH	C6-C5-C10	-2.85	109.59	112.67
3	A	601	TCH	C19-C10-C5	2.85	115.18	110.26
3	B	602	TCH	C5-C4-C3	-2.77	108.88	112.95
3	A	601	TCH	O3-C3-C2	2.72	117.94	110.04
3	B	601	TCH	O3-C3-C2	2.70	117.88	110.04
3	A	602	TCH	C1-C10-C9	-2.69	107.14	111.45
3	A	602	TCH	C14-C8-C7	2.66	115.10	111.81
3	B	602	TCH	C19-C10-C5	2.65	114.84	110.26
3	A	602	TCH	C19-C10-C5	2.65	114.83	110.26
3	B	601	TCH	C6-C5-C10	-2.60	109.86	112.67
3	B	601	TCH	C21-C20-C17	-2.59	108.42	112.96
3	A	602	TCH	O3-C3-C2	2.59	117.54	110.04
3	B	601	TCH	C19-C10-C5	2.56	114.69	110.26
3	A	601	TCH	C4-C5-C10	-2.55	109.92	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	TCH	C25-C26-S26	-2.54	107.02	113.66
3	A	601	TCH	C22-C20-C17	2.53	115.93	110.25
3	A	601	TCH	C19-C10-C9	-2.53	107.90	111.17
3	A	602	TCH	C15-C16-C17	2.52	110.26	105.14
3	B	602	TCH	C1-C10-C5	2.49	110.54	107.79
3	B	602	TCH	C9-C10-C5	-2.45	105.27	108.67
3	B	602	TCH	C15-C16-C17	2.39	109.99	105.14
3	A	601	TCH	O7-C7-C6	2.38	115.88	110.09
3	A	602	TCH	C6-C7-C8	2.34	113.99	111.51
3	B	601	TCH	C1-C10-C5	2.29	110.32	107.79
3	B	602	TCH	O7-C7-C6	2.25	115.57	110.09
3	B	602	TCH	O3-C3-C2	2.22	116.47	110.04
3	A	602	TCH	C14-C13-C12	-2.19	105.38	107.40
3	A	601	TCH	C21-C20-C17	-2.18	109.15	112.96
3	B	601	TCH	C6-C7-C8	2.17	113.81	111.51
3	A	602	TCH	C9-C8-C7	-2.17	109.55	111.97
3	A	602	TCH	C19-C10-C9	-2.12	108.43	111.17

All (16) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.