



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM 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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

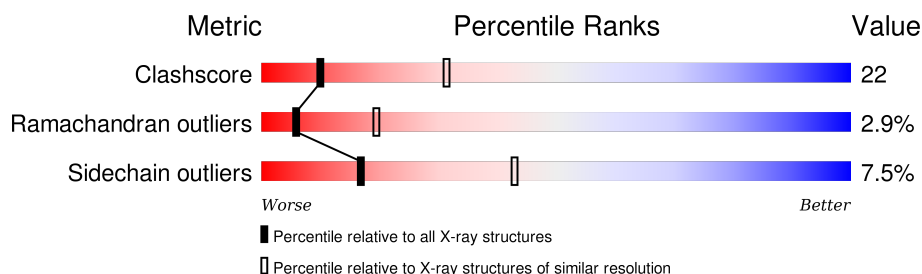
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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. 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.

Note EDS was not executed.

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

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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TCH	B	602	X	-	-	-

2 Entry composition [i](#)

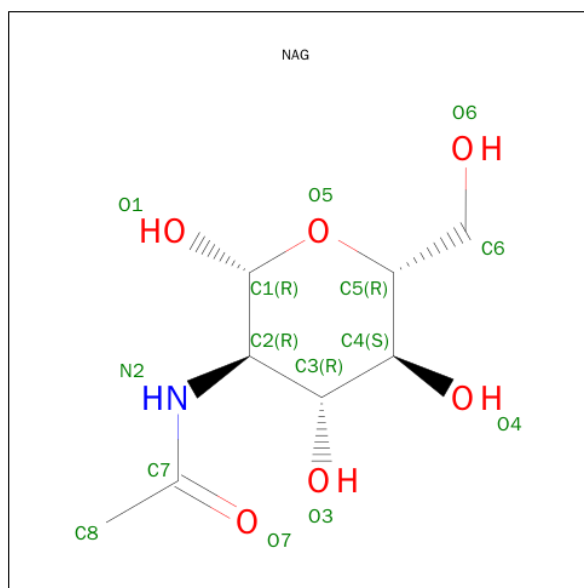
There are 3 unique types of molecules in this entry. The entry contains 8498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

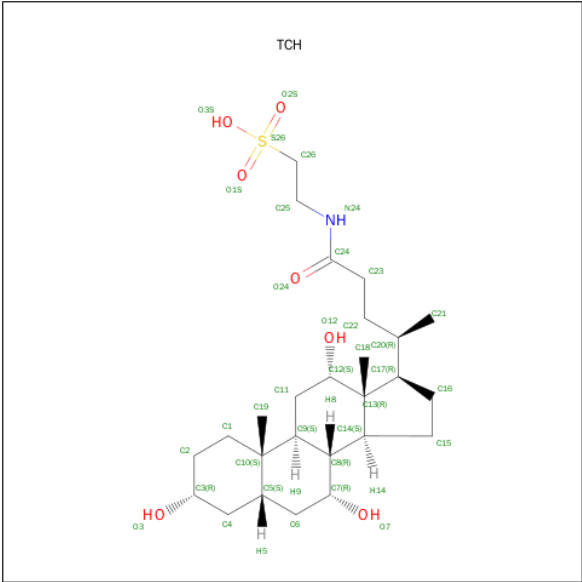
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			
1	B	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			

- 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: $C_{26}H_{45}NO_7S$).



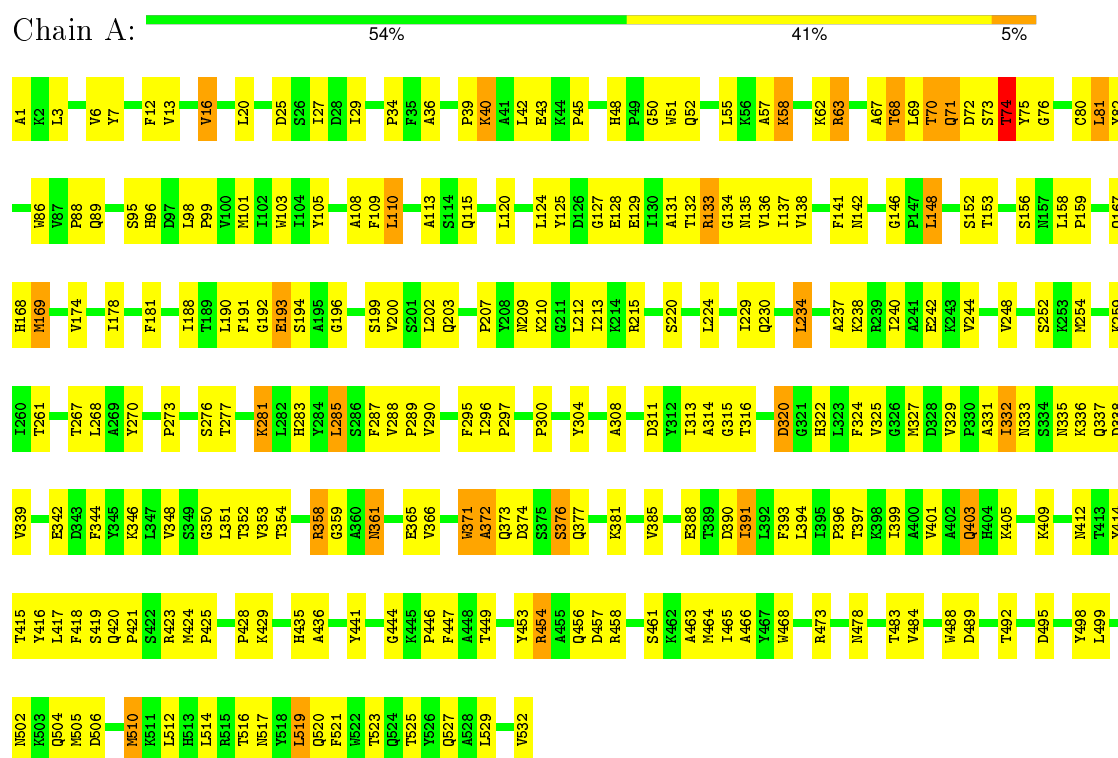
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		

3 Residue-property plots

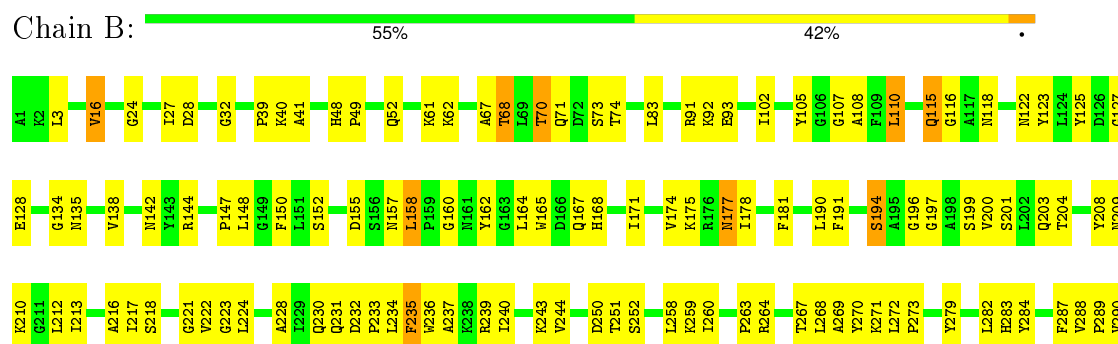
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



• Molecule 1: BILE-SALT ACTIVATED LIPASE



T825	Q440	E365	I291
Y526	Y441	E369	D294
Q527	Y442	E370	F295
P530	F443	P371	I296
	G444	P372	P297
T831	K445	A372	D298
V532	P446	Q373	D299
	F447	D374	P300
	A448	I375	V301
T449	T449	Q377	N302
P450	P450	R380	I303
L451	L451	A381	Y304
	G452	K382	A308
Y453	R454	T383	D309
A455	A455	P384	V310
Q456	Q456	V385	I313
D457	D457	D386	A314
R458	R458	E387	D318
T459	T459	T388	K319
P460	P460	T389	D320
K462	K462	L392	G321
	I465	F393	H322
	W468	L394	
T469	T469	I395	V325
		T397	P330
R473	R473	K398	A331
T474	T474	I399	I332
		A400	N333
T483	T483	V401	S334
			N335
D489	D489	H404	K336
P490	P490		Q337
E494	E494	A408	D338
D495	D495	K409	V339
D496	D496	W412	T340
W497	W497	T413	F341
Y498	Y498	Y414	E342
		T415	D343
K503	K503	Y416	
Q504	Q504	L417	K346
S507	S507	R423	G350
		M424	L351
M510	M510		T352
K511	K511	Y427	K355
L512	L512	P428	G356
H513	H513	K429	L357
L514	L514	W430	R358
R515	R515	M431	G359
L519	L519	H435	A360
F520	F520	A436	N361
Q521	Q521	D437	A362
W522	W522	T438	T363
		L439	V364

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 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: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
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

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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: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
1:B:39:PRO:HB2	1:B:144:ARG:NH1	2.18	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: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	Interatomic distance (Å)	Clash overlap (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

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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: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

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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: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

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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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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%)	5	18
1	B	530/532 (100%)	456 (86%)	59 (11%)	15 (3%)	6	21
All	All	1060/1064 (100%)	907 (86%)	122 (12%)	31 (3%)	6	19

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 ⓘ

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%)	11	32
1	B	444/444 (100%)	418 (94%)	26 (6%)	24	57
All	All	888/888 (100%)	821 (92%)	67 (8%)	17	43

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

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 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 ⓘ

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	14,14,15	0.69	0	15,19,21	1.00	1 (6%)
3	TCH	A	601	-	37,38,38	2.09	11 (29%)	59,60,60	4.85	37 (62%)
3	TCH	A	602	-	37,38,38	2.20	12 (32%)	59,60,60	4.96	37 (62%)
2	NAG	B	600	1	14,14,15	0.70	0	15,19,21	1.11	2 (13%)
3	TCH	B	601	-	37,38,38	2.07	11 (29%)	59,60,60	4.75	35 (59%)
3	TCH	B	602	-	37,38,38	1.97	10 (27%)	59,60,60	4.75	36 (61%)

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	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TCH	A	602	-	4/4/13/14	0/16/81/81	0/4/4/4
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	0/4/4/4
3	TCH	B	602	-	4/4/13/14	0/16/81/81	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	TCH	C6-C5	-5.28	1.44	1.53
3	A	602	TCH	C6-C5	-5.06	1.45	1.53
3	A	602	TCH	C10-C5	-5.00	1.46	1.55
3	B	602	TCH	C11-C9	-4.71	1.46	1.53
3	B	602	TCH	C10-C5	-4.41	1.47	1.55
3	A	602	TCH	C6-C7	-4.29	1.45	1.52
3	A	602	TCH	C11-C9	-4.18	1.46	1.53
3	B	602	TCH	C10-C9	-4.16	1.47	1.56
3	A	602	TCH	C8-C7	-4.14	1.46	1.53
3	B	601	TCH	C10-C5	-3.89	1.48	1.55
3	B	601	TCH	C11-C9	-3.72	1.47	1.53
3	A	601	TCH	C11-C9	-3.60	1.47	1.53
3	A	601	TCH	C10-C5	-3.24	1.49	1.55
3	B	601	TCH	C6-C7	-3.15	1.47	1.52
3	A	602	TCH	C21-C20	-3.11	1.45	1.53
3	A	602	TCH	C8-C14	-2.46	1.48	1.53
3	A	601	TCH	C6-C5	-2.41	1.49	1.53
3	A	602	TCH	C10-C9	-2.34	1.51	1.56
3	B	602	TCH	C21-C20	-2.12	1.47	1.53
3	B	601	TCH	C21-C20	-2.06	1.47	1.53
3	B	601	TCH	C19-C10	-2.01	1.50	1.54
3	A	601	TCH	C13-C12	2.08	1.57	1.54
3	A	602	TCH	C11-C12	2.12	1.57	1.53
3	B	601	TCH	C22-C23	2.25	1.60	1.52
3	A	602	TCH	C8-C9	2.33	1.58	1.53
3	B	602	TCH	O12-C12	2.60	1.48	1.43
3	B	601	TCH	C18-C13	2.63	1.58	1.54
3	A	602	TCH	C18-C13	2.64	1.58	1.54
3	A	601	TCH	C8-C14	2.65	1.59	1.53
3	B	601	TCH	O24-C24	2.72	1.29	1.23
3	A	601	TCH	C24-N24	2.81	1.40	1.33
3	B	602	TCH	O24-C24	2.82	1.29	1.23
3	A	601	TCH	C13-C17	2.82	1.60	1.55
3	B	602	TCH	C8-C7	2.97	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	TCH	C4-C3	2.99	1.57	1.51
3	A	602	TCH	O24-C24	3.10	1.29	1.23
3	B	601	TCH	C8-C9	3.15	1.60	1.53
3	B	602	TCH	C6-C7	3.22	1.58	1.52
3	A	601	TCH	O24-C24	3.40	1.30	1.23
3	A	601	TCH	C18-C13	3.84	1.60	1.54
3	A	601	TCH	C20-C17	3.86	1.61	1.54
3	B	602	TCH	C18-C13	3.86	1.60	1.54
3	B	601	TCH	C11-C12	4.08	1.60	1.53
3	A	601	TCH	C8-C9	4.87	1.63	1.53

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TCH	C9-C11-C12	-11.27	100.12	114.36
3	A	601	TCH	C9-C11-C12	-10.88	100.62	114.36
3	A	602	TCH	C9-C11-C12	-10.06	101.65	114.36
3	B	601	TCH	C9-C11-C12	-8.66	103.42	114.36
3	A	602	TCH	C5-C6-C7	-8.26	105.22	114.44
3	B	601	TCH	C5-C6-C7	-6.10	107.64	114.44
3	B	602	TCH	C17-C13-C14	-5.82	94.17	100.05
3	A	602	TCH	C17-C13-C14	-5.57	94.43	100.05
3	B	601	TCH	C17-C13-C14	-5.20	94.80	100.05
3	A	601	TCH	C17-C13-C14	-5.03	94.97	100.05
3	B	601	TCH	C13-C14-C8	-4.95	108.37	114.75
3	B	601	TCH	C4-C3-C2	-4.94	104.22	110.52
3	A	602	TCH	C5-C4-C3	-4.75	105.85	112.91
3	B	602	TCH	C9-C8-C7	-4.64	106.44	111.92
3	B	601	TCH	O24-C24-N24	-4.61	113.78	122.94
3	A	602	TCH	C4-C3-C2	-4.60	104.65	110.52
3	A	601	TCH	O24-C24-N24	-4.60	113.81	122.94
3	A	601	TCH	C4-C3-C2	-4.60	104.66	110.52
3	B	602	TCH	O1S-S26-C26	-4.52	103.05	106.91
3	B	602	TCH	O24-C24-N24	-4.39	114.22	122.94
3	A	601	TCH	O1S-S26-C26	-4.32	103.22	106.91
3	A	601	TCH	C14-C13-C12	-4.11	103.71	107.39
3	B	601	TCH	C18-C13-C14	-4.09	104.76	111.22
3	A	601	TCH	C13-C14-C8	-4.03	109.56	114.75
3	B	601	TCH	C5-C4-C3	-3.98	107.00	112.91
3	A	601	TCH	C18-C13-C14	-3.93	105.02	111.22
3	A	602	TCH	O24-C24-N24	-3.92	115.15	122.94
3	B	602	TCH	C4-C5-C10	-3.79	108.48	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TCH	C18-C13-C14	-3.74	105.31	111.22
3	B	601	TCH	O1S-S26-C26	-3.64	103.80	106.91
3	B	602	TCH	C16-C15-C14	-3.61	97.85	105.12
3	A	602	TCH	C13-C14-C8	-3.61	110.10	114.75
3	B	602	TCH	C13-C14-C8	-3.58	110.14	114.75
3	B	602	TCH	C25-C26-S26	-3.57	104.10	113.73
3	A	602	TCH	C25-C26-S26	-3.56	104.12	113.73
3	A	601	TCH	C25-C26-S26	-3.50	104.30	113.73
3	A	602	TCH	C16-C15-C14	-3.38	98.32	105.12
3	A	602	TCH	O1S-S26-C26	-3.35	104.05	106.91
3	B	602	TCH	C18-C13-C14	-3.26	106.07	111.22
3	A	602	TCH	C21-C20-C17	-3.26	107.53	112.96
3	A	601	TCH	C5-C4-C3	-3.14	108.25	112.91
3	A	601	TCH	C16-C15-C14	-2.97	99.13	105.12
3	B	602	TCH	C4-C3-C2	-2.95	106.76	110.52
3	B	601	TCH	C16-C15-C14	-2.90	99.28	105.12
3	A	601	TCH	C5-C6-C7	-2.90	111.21	114.44
3	A	602	TCH	C6-C5-C10	-2.78	109.59	112.66
3	B	601	TCH	C21-C20-C17	-2.72	108.42	112.96
3	B	602	TCH	C5-C4-C3	-2.71	108.88	112.91
3	A	602	TCH	C1-C10-C9	-2.67	107.14	111.45
3	B	601	TCH	C6-C5-C10	-2.54	109.86	112.66
3	B	601	TCH	C25-C26-S26	-2.49	107.02	113.73
3	A	601	TCH	C4-C5-C10	-2.49	109.92	112.66
3	B	602	TCH	C9-C10-C5	-2.30	105.27	108.67
3	A	601	TCH	C21-C20-C17	-2.28	109.15	112.96
3	B	601	TCH	O24-C24-C23	-2.28	118.05	121.98
3	A	602	TCH	C14-C13-C12	-2.25	105.38	107.39
3	B	602	TCH	O24-C24-C23	-2.20	118.19	121.98
3	A	601	TCH	C19-C10-C9	-2.19	107.90	111.18
3	A	601	TCH	O24-C24-C23	-2.12	118.32	121.98
3	A	602	TCH	O24-C24-C23	-2.08	118.39	121.98
2	B	600	NAG	C8-C7-N2	-2.01	112.26	116.11
3	A	602	TCH	C9-C8-C7	-2.01	109.55	111.92
3	B	602	TCH	C16-C17-C20	2.07	115.74	112.05
3	B	601	TCH	C22-C20-C17	2.10	114.65	110.24
2	A	600	NAG	C1-O5-C5	2.15	114.97	112.25
3	B	601	TCH	C6-C7-C8	2.20	113.81	111.47
3	B	602	TCH	O7-C7-C6	2.25	115.57	110.06
3	B	602	TCH	O3-C3-C2	2.27	116.47	110.05
3	A	602	TCH	C6-C7-C8	2.37	113.99	111.47
3	A	601	TCH	O7-C7-C6	2.37	115.88	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TCH	C15-C16-C17	2.42	109.99	105.12
3	A	602	TCH	C14-C8-C7	2.42	115.10	111.74
3	B	601	TCH	C19-C10-C5	2.51	114.69	110.25
3	A	602	TCH	C15-C16-C17	2.55	110.26	105.12
2	B	600	NAG	C1-O5-C5	2.59	115.53	112.25
3	A	602	TCH	C19-C10-C5	2.59	114.83	110.25
3	B	602	TCH	C19-C10-C5	2.60	114.84	110.25
3	A	602	TCH	O3-C3-C2	2.65	117.54	110.05
3	A	601	TCH	C22-C20-C17	2.71	115.93	110.24
3	B	601	TCH	O3-C3-C2	2.77	117.88	110.05
3	A	601	TCH	O3-C3-C2	2.79	117.94	110.05
3	A	601	TCH	C19-C10-C5	2.79	115.18	110.25
3	A	602	TCH	C23-C22-C20	2.82	119.59	114.48
3	B	601	TCH	C15-C16-C17	2.91	110.99	105.12
3	A	601	TCH	C15-C16-C17	2.94	111.05	105.12
3	A	602	TCH	C26-C25-N24	3.09	120.77	111.27
3	B	602	TCH	C26-C25-N24	3.16	120.98	111.27
3	B	602	TCH	C6-C7-C8	3.18	114.84	111.47
3	A	601	TCH	C23-C22-C20	3.21	120.30	114.48
3	A	601	TCH	C26-C25-N24	3.33	121.49	111.27
3	B	601	TCH	C23-C22-C20	3.41	120.65	114.48
3	B	601	TCH	C14-C8-C9	3.52	114.47	109.62
3	B	601	TCH	C26-C25-N24	3.61	122.37	111.27
3	B	602	TCH	C23-C22-C20	3.69	121.15	114.48
3	B	602	TCH	C10-C9-C8	3.79	116.04	111.88
3	A	602	TCH	C14-C8-C9	3.98	115.10	109.62
3	B	601	TCH	C14-C8-C7	4.41	117.86	111.74
3	B	602	TCH	C13-C17-C20	4.42	124.89	119.50
3	A	601	TCH	C14-C8-C7	4.46	117.93	111.74
3	A	601	TCH	C14-C8-C9	4.49	115.80	109.62
3	B	602	TCH	C11-C12-C13	4.81	116.09	111.20
3	A	602	TCH	C15-C14-C8	4.83	125.33	118.32
3	A	601	TCH	C6-C5-C4	4.90	116.51	111.05
3	B	602	TCH	C14-C8-C7	5.08	118.78	111.74
3	B	602	TCH	C14-C8-C9	5.09	116.62	109.62
3	B	602	TCH	C16-C17-C13	5.16	108.73	103.60
3	B	601	TCH	C13-C17-C20	5.29	125.94	119.50
3	A	601	TCH	C16-C17-C13	5.31	108.89	103.60
3	B	601	TCH	C15-C14-C8	5.32	126.04	118.32
3	A	602	TCH	C16-C17-C13	5.57	109.13	103.60
3	A	602	TCH	C13-C17-C20	5.65	126.38	119.50
3	B	602	TCH	C6-C5-C4	5.74	117.46	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	TCH	C15-C14-C8	5.88	126.86	118.32
3	B	602	TCH	O3-C3-C4	5.98	121.76	109.86
3	A	602	TCH	C11-C12-C13	6.11	117.41	111.20
3	B	601	TCH	C6-C5-C4	6.15	117.91	111.05
3	B	601	TCH	C16-C17-C13	6.21	109.77	103.60
3	A	601	TCH	C11-C12-C13	6.29	117.59	111.20
3	B	602	TCH	C15-C14-C8	6.31	127.49	118.32
3	B	602	TCH	C18-C13-C12	6.33	115.27	109.09
3	B	601	TCH	C18-C13-C12	6.35	115.28	109.09
3	A	601	TCH	O3-C3-C4	6.45	122.68	109.86
3	A	602	TCH	O3-C3-C4	6.46	122.72	109.86
3	A	601	TCH	O12-C12-C11	6.51	122.39	109.06
3	A	601	TCH	C13-C17-C20	6.59	127.52	119.50
3	B	601	TCH	O3-C3-C4	6.66	123.10	109.86
3	A	601	TCH	C10-C9-C8	6.67	119.20	111.88
3	A	602	TCH	O12-C12-C11	7.08	123.55	109.06
3	A	602	TCH	C18-C13-C12	7.13	116.05	109.09
3	B	601	TCH	O12-C12-C11	7.19	123.78	109.06
3	A	602	TCH	C6-C5-C4	7.39	119.30	111.05
3	B	602	TCH	O12-C12-C11	7.48	124.38	109.06
3	B	601	TCH	C10-C9-C8	7.51	120.12	111.88
3	A	602	TCH	C10-C9-C8	7.68	120.31	111.88
3	A	601	TCH	C18-C13-C12	7.79	116.68	109.09
3	B	601	TCH	C11-C12-C13	7.95	119.28	111.20
3	B	601	TCH	C11-C9-C8	11.93	127.70	110.73
3	A	602	TCH	C11-C9-C8	12.05	127.86	110.73
3	A	601	TCH	C11-C9-C8	12.24	128.13	110.73
3	B	602	TCH	C15-C14-C13	12.79	116.33	103.60
3	A	601	TCH	C15-C14-C13	13.54	117.06	103.60
3	B	602	TCH	C11-C9-C8	13.72	130.24	110.73
3	B	601	TCH	O2S-S26-C26	13.99	118.84	106.91
3	B	601	TCH	C15-C14-C13	14.08	117.61	103.60
3	A	602	TCH	C15-C14-C13	14.60	118.12	103.60
3	B	602	TCH	O2S-S26-C26	15.37	120.02	106.91
3	A	602	TCH	O2S-S26-C26	16.03	120.58	106.91
3	A	601	TCH	O2S-S26-C26	16.06	120.61	106.91

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	602	TCH	C5
3	B	602	TCH	C3

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Mol	Chain	Res	Type	Atom
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.

6 monomers are involved in 23 short contacts:

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

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.