



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:07 AM UTC

PDB ID : 1AQL / pdb_00001aql
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

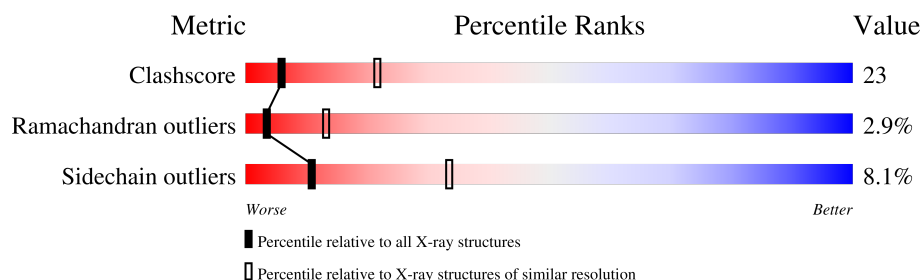
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

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	-	-	-
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.

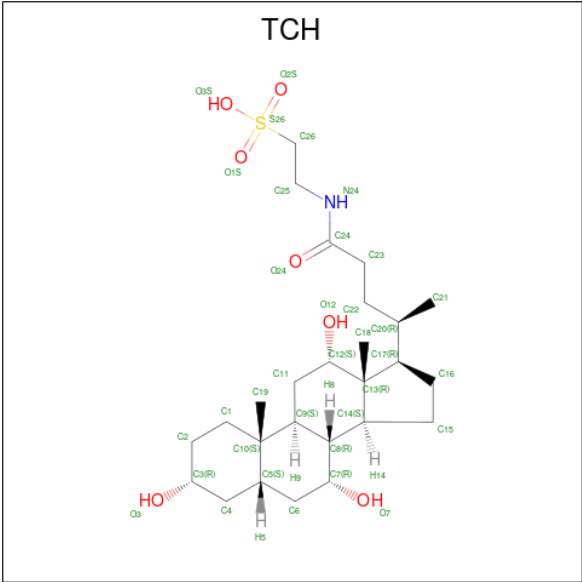
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			
1	B	532	Total	C	N	O	S	0	0	0
			4165	2668	692	788	17			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: TCH) (formula: $C_{26}H_{45}NO_7S$).



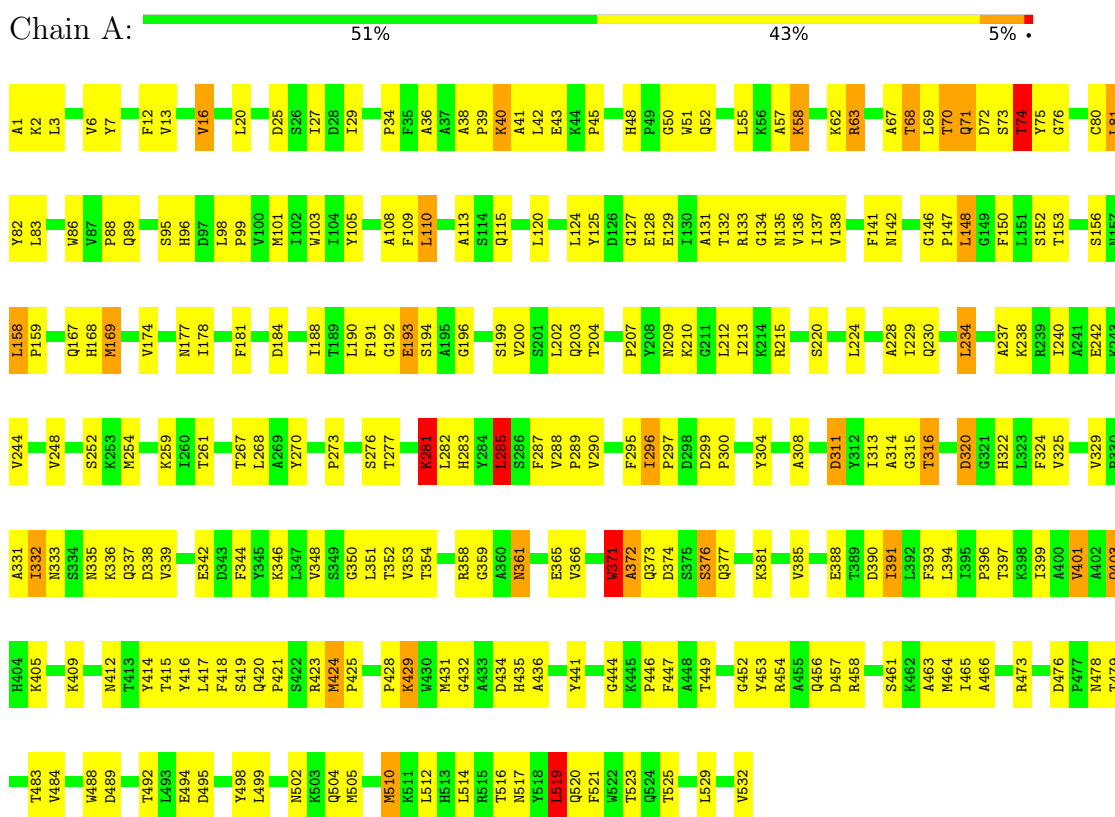
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	A	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		
3	B	1	Total	C	N	O	S	0	0
			35	26	1	7	1		

3 Residue-property plots

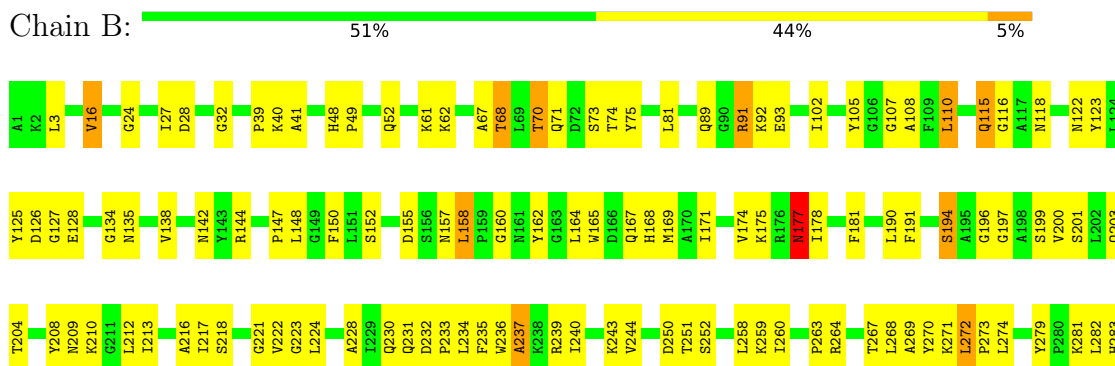
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

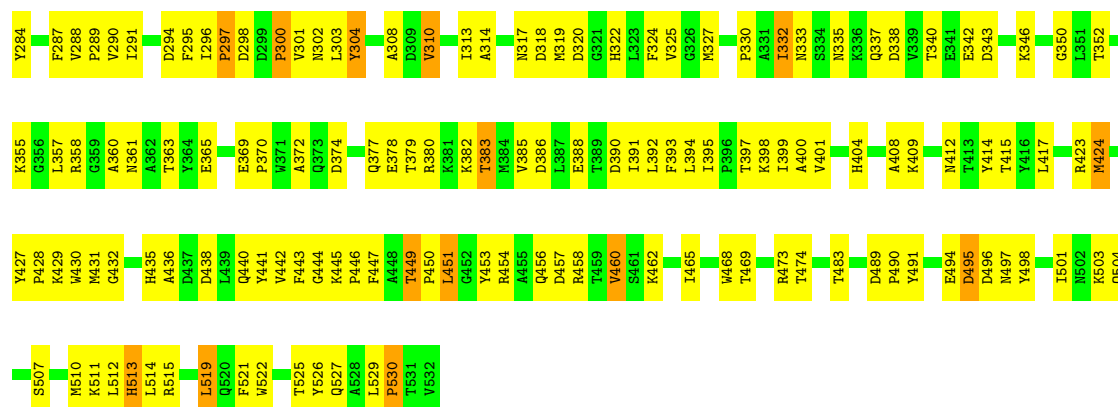
Note EDS was not executed.

- Molecule 1: BILE-SALT ACTIVATED LIPASE



- Molecule 1: BILE-SALT ACTIVATED LIPASE





4 Data and refinement statistics

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

5.1 Standard geometry

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	0.57	0/4278	1.05	21/5824 (0.4%)
1	B	0.55	0/4278	1.05	21/5824 (0.4%)
All	All	0.56	0/8556	1.05	42/11648 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	LEU	CA-C-N	7.41	128.06	119.47
1	A	158	LEU	C-N-CA	7.41	128.06	119.47
1	B	495	ASP	N-CA-C	7.39	119.41	111.36
1	B	449	THR	CA-C-N	7.36	127.71	119.32
1	B	449	THR	C-N-CA	7.36	127.71	119.32
1	A	177	ASN	N-CA-C	7.03	120.51	112.57
1	B	393	PHE	N-CA-C	6.97	121.46	112.12
1	B	237	ALA	N-CA-C	-6.74	103.85	111.07
1	A	479	THR	N-CA-C	6.46	119.47	109.07
1	B	496	ASP	N-CA-C	-6.45	102.49	111.52
1	A	296	ILE	CA-C-N	6.37	125.59	118.97
1	A	296	ILE	C-N-CA	6.37	125.59	118.97
1	A	38	ALA	CA-C-N	6.37	126.34	119.78
1	A	38	ALA	C-N-CA	6.37	126.34	119.78
1	A	519	LEU	N-CA-C	-6.32	104.39	111.28
1	A	424	MET	CA-C-N	6.28	127.09	120.12
1	A	424	MET	C-N-CA	6.28	127.09	120.12
1	B	89	GLN	N-CA-C	6.25	119.59	109.40
1	A	299	ASP	N-CA-C	-6.23	101.92	109.83
1	B	272	LEU	CA-C-N	6.13	127.50	119.84
1	B	272	LEU	C-N-CA	6.13	127.50	119.84
1	A	285	LEU	N-CA-C	-6.00	101.02	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ASN	N-CA-C	5.94	120.96	111.81
1	A	150	PHE	N-CA-C	5.92	119.74	111.56
1	A	184	ASP	CA-C-N	5.84	125.31	119.24
1	A	184	ASP	C-N-CA	5.84	125.31	119.24
1	B	460	VAL	N-CA-C	-5.81	104.67	110.30
1	B	424	MET	CA-C-N	5.77	125.47	119.64
1	B	424	MET	C-N-CA	5.77	125.47	119.64
1	B	529	LEU	CA-C-N	5.73	127.00	119.84
1	B	529	LEU	C-N-CA	5.73	127.00	119.84
1	B	501	ILE	N-CA-C	5.67	116.02	107.80
1	B	91	ARG	N-CA-C	5.61	117.84	111.11
1	B	126	ASP	N-CA-C	-5.51	101.70	109.96
1	A	228	ALA	N-CA-C	5.50	119.70	113.15
1	A	371	TRP	N-CA-C	5.22	116.75	108.96
1	A	311	ASP	N-CA-C	-5.19	103.49	110.24
1	B	317	ASN	N-CA-C	-5.19	100.72	109.07
1	A	452	GLY	N-CA-C	-5.12	108.05	115.27
1	B	304	TYR	N-CA-C	5.11	119.01	112.87
1	A	361	ASN	CB-CG-ND2	5.06	123.99	116.40
1	B	378	GLU	N-CA-C	-5.04	105.79	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4165	0	4055	205	0
1	B	4165	0	4055	176	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	384	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 23.

All (384) 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:45:PRO:HG2	1:A:169:MET:HE2	1.54	0.89
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:B:489:ASP:HB2	1:B:510:MET:HE2	1.68	0.74
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:A:338:ASP:HA	1:A:381:LYS:HZ1	1.53	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:274:LEU:HA	1:B:281:LYS:HZ1	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:333:ASN:C	1:A:335:ASN:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:338:ASP:HB2	1:B:377:GLN:CD	2.34	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: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:238:LYS:HA	1:A:254:MET:HE1	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:391:ILE:HG13	1:B:392:LEU:N	2.26	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:324:PHE:HA	1:B:327:MET:HE3	1.95	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: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:A:431:MET:HE2	1:A:434:ASP:HB2	1.96	0.47
1:A:456:GLN:CD	1:A:456:GLN:H	2.22	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:C	1:B:260:ILE:H	2.22	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
1:A:58:LYS:HD3	1:A:58:LYS:C	2.39	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
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:333:ASN:C	1:A:335:ASN:N	2.72	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: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:B:40:LYS:O	1:B:41:ALA:C	2.57	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: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:449:THR:HG21	3:B:601:TCH:HO7	1.81	0.45
1:B:497:ASN:HB3	1:B:512:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:40:LYS:O	1:A:41:ALA:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:409:LYS:HB3	1:A:409:LYS:HZ3	1.80	0.44
1:B:16:VAL:O	1:B:28:ASP:HA	2.18	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
1:A:494:GLU:CD	1:A:494:GLU:H	2.27	0.43
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:A:405:LYS:HZ2	1:A:492:THR:HA	1.81	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:339:VAL:H	1:A:381:LYS:HZ2	1.65	0.43
1:B:491:TYR:CD1	1:B:491:TYR:C	2.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:338:ASP:HA	1:A:381:LYS:NZ	2.29	0.42
1:A:72:ASP:C	1:A:74:THR:H	2.27	0.42
1:A:431:MET:HE3	1:A:432:GLY:O	2.20	0.42
1:B:204:THR:CG2	1:B:310:VAL:HG11	2.50	0.42
1:A:215:ARG:HD3	1:A:311:ASP:HB2	2.02	0.41
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: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:B:73:SER:C	1:B:75:TYR:H	2.28	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:83:LEU:HD12	1:A:83:LEU:C	2.45	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:A:476:ASP:C	1:A:478:ASN:H	2.29	0.41
1:B:108:ALA:C	1:B:110:LEU:H	2.28	0.41
1:B:489:ASP:HA	1:B:490:PRO:HD3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:MET:HE3	1:B:432:GLY:H	1.86	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
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%)	3	12
1	B	530/532 (100%)	456 (86%)	59 (11%)	15 (3%)	4	14
All	All	1060/1064 (100%)	907 (86%)	122 (12%)	31 (3%)	3	13

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
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%)	8 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	444/444 (100%)	413 (93%)	31 (7%)	14	40
All	All	888/888 (100%)	816 (92%)	72 (8%)	11	33

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
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	147	PRO
1	A	148	LEU
1	A	169	MET
1	A	193	GLU
1	A	204	THR
1	A	234	LEU
1	A	252	SER
1	A	261	THR
1	A	277	THR
1	A	281	LYS
1	A	282	LEU
1	A	285	LEU
1	A	316	THR
1	A	320	ASP
1	A	329	VAL
1	A	365	GLU
1	A	371	TRP
1	A	376	SER
1	A	391	ILE
1	A	401	VAL
1	A	403	GLN
1	A	423	ARG
1	A	429	LYS
1	A	483	THR

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Mol	Chain	Res	Type
1	A	504	GLN
1	A	510	MET
1	A	516	THR
1	A	519	LEU
1	A	532	VAL
1	B	16	VAL
1	B	68	THR
1	B	71	GLN
1	B	74	THR
1	B	81	LEU
1	B	110	LEU
1	B	115	GLN
1	B	169	MET
1	B	177	ASN
1	B	194	SER
1	B	201	SER
1	B	234	LEU
1	B	250	ASP
1	B	263	PRO
1	B	282	LEU
1	B	300	PRO
1	B	310	VAL
1	B	319	MET
1	B	320	ASP
1	B	332	ILE
1	B	379	THR
1	B	383	THR
1	B	423	ARG
1	B	429	LYS
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	84	ASN

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Mol	Chain	Res	Type
1	A	157	ASN
1	A	168	HIS
1	A	231	GLN
1	A	283	HIS
1	A	335	ASN
1	A	420	GLN
1	A	513	HIS
1	A	520	GLN
1	A	524	GLN
1	B	17	ASN
1	B	84	ASN
1	B	115	GLN
1	B	157	ASN
1	B	168	HIS
1	B	177	ASN
1	B	230	GLN
1	B	231	GLN
1	B	283	HIS
1	B	481	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 oligosaccharides 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
3	TCH	B	601	-	38,38,38	2.19	14 (36%)	59,60,60	4.48	34 (57%)
3	TCH	A	602	-	38,38,38	2.27	16 (42%)	59,60,60	4.60	35 (59%)
2	NAG	B	600	1	14,14,15	0.75	0	17,19,21	1.12	3 (17%)
2	NAG	A	600	1	14,14,15	0.72	0	17,19,21	0.99	2 (11%)
3	TCH	B	602	-	38,38,38	2.04	12 (31%)	59,60,60	4.38	35 (59%)
3	TCH	A	601	-	38,38,38	2.19	14 (36%)	59,60,60	4.49	37 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TCH	B	601	-	4/4/13/14	10/16/81/81	0/4/4/4
3	TCH	A	602	-	4/4/13/14	8/16/81/81	0/4/4/4
2	NAG	B	600	1	-	2/6/23/26	0/1/1/1
2	NAG	A	600	1	-	2/6/23/26	0/1/1/1
3	TCH	B	602	-	4/4/13/14	11/16/81/81	0/4/4/4
3	TCH	A	601	-	4/4/13/14	9/16/81/81	0/4/4/4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	TCH	C6-C5	-5.77	1.44	1.53
3	A	602	TCH	C6-C5	-5.52	1.45	1.53
3	A	602	TCH	C10-C5	-5.46	1.46	1.55
3	A	601	TCH	C8-C9	4.99	1.63	1.53
3	B	602	TCH	C10-C5	-4.82	1.47	1.55
3	B	602	TCH	C11-C9	-4.81	1.46	1.53
3	B	602	TCH	C10-C9	-4.66	1.47	1.56
3	B	601	TCH	C11-C12	4.61	1.60	1.53
3	A	602	TCH	C11-C9	-4.26	1.46	1.53
3	B	601	TCH	C10-C5	-4.26	1.48	1.55
3	A	601	TCH	C20-C17	4.23	1.61	1.54
3	B	602	TCH	C18-C13	3.99	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	TCH	C18-C13	3.98	1.60	1.54
3	B	601	TCH	C11-C9	-3.79	1.47	1.53
3	A	602	TCH	C8-C7	-3.75	1.46	1.53
3	A	601	TCH	C11-C9	-3.67	1.47	1.53
3	A	602	TCH	C6-C7	-3.63	1.45	1.52
3	A	601	TCH	O24-C24	3.60	1.30	1.23
3	A	601	TCH	C10-C5	-3.55	1.49	1.55
3	A	602	TCH	O24-C24	3.29	1.29	1.23
3	B	601	TCH	C8-C9	3.22	1.60	1.53
3	B	602	TCH	C4-C3	3.15	1.57	1.52
3	A	602	TCH	C21-C20	-3.13	1.45	1.53
3	A	601	TCH	C13-C17	3.00	1.60	1.55
3	B	602	TCH	O24-C24	2.99	1.29	1.23
3	B	601	TCH	O24-C24	2.88	1.29	1.23
3	A	601	TCH	C24-N24	2.84	1.40	1.33
3	B	602	TCH	O12-C12	2.78	1.48	1.43
3	B	602	TCH	C6-C7	2.76	1.58	1.52
3	A	602	TCH	C18-C13	2.74	1.58	1.54
3	B	601	TCH	C18-C13	2.73	1.58	1.54
3	A	601	TCH	C8-C14	2.70	1.59	1.53
3	B	602	TCH	C8-C7	2.67	1.58	1.53
3	B	601	TCH	C6-C7	-2.66	1.47	1.52
3	A	601	TCH	C6-C5	-2.65	1.49	1.53
3	A	602	TCH	C10-C9	-2.60	1.51	1.56
3	A	602	TCH	C8-C14	-2.58	1.48	1.53
3	B	601	TCH	C22-C23	2.44	1.60	1.52
3	A	602	TCH	C11-C12	2.43	1.57	1.53
3	A	602	TCH	C8-C9	2.37	1.58	1.53
3	B	601	TCH	C2-C3	-2.27	1.46	1.51
3	A	601	TCH	C11-C12	2.25	1.56	1.53
3	B	601	TCH	C19-C10	-2.23	1.50	1.54
3	A	602	TCH	C26-S26	-2.22	1.74	1.77
3	B	601	TCH	C26-S26	2.20	1.80	1.77
3	A	602	TCH	C4-C5	-2.16	1.50	1.53
3	A	601	TCH	C22-C23	2.15	1.59	1.52
3	B	602	TCH	C21-C20	-2.14	1.47	1.53
3	A	601	TCH	C13-C12	2.12	1.57	1.54
3	A	601	TCH	O12-C12	2.08	1.47	1.43
3	A	602	TCH	C20-C17	-2.08	1.50	1.54
3	B	601	TCH	C21-C20	-2.07	1.47	1.53
3	B	601	TCH	C22-C20	2.06	1.59	1.54
3	B	602	TCH	C1-C10	-2.03	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	TCH	O1S-S26	-2.02	1.39	1.45
3	B	602	TCH	C6-C5	2.00	1.57	1.53

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TCH	C15-C14-C13	15.03	118.12	103.54
3	B	601	TCH	C15-C14-C13	14.50	117.61	103.54
3	A	601	TCH	C15-C14-C13	13.94	117.06	103.54
3	B	602	TCH	C15-C14-C13	13.18	116.33	103.54
3	B	602	TCH	C11-C9-C8	13.07	130.24	110.89
3	A	601	TCH	C11-C9-C8	11.65	128.13	110.89
3	A	602	TCH	C11-C9-C8	11.46	127.86	110.89
3	B	601	TCH	C11-C9-C8	11.35	127.70	110.89
3	B	602	TCH	C9-C11-C12	-10.83	100.12	114.29
3	A	601	TCH	C9-C11-C12	-10.45	100.62	114.29
3	A	602	TCH	C9-C11-C12	-9.66	101.65	114.29
3	A	601	TCH	O2S-S26-C26	9.19	120.61	106.73
3	A	602	TCH	O2S-S26-C26	9.17	120.58	106.73
3	B	602	TCH	O2S-S26-C26	8.79	120.02	106.73
3	B	601	TCH	C9-C11-C12	-8.31	103.42	114.29
3	B	601	TCH	O2S-S26-C26	8.02	118.84	106.73
3	B	601	TCH	C11-C12-C13	7.88	119.28	111.26
3	A	602	TCH	C5-C6-C7	-7.72	105.22	114.40
3	A	601	TCH	C18-C13-C12	7.62	116.68	109.06
3	A	602	TCH	C10-C9-C8	7.60	120.31	111.84
3	B	602	TCH	O12-C12-C11	7.50	124.38	109.12
3	B	601	TCH	C10-C9-C8	7.43	120.12	111.84
3	B	601	TCH	O12-C12-C11	7.20	123.78	109.12
3	A	602	TCH	O12-C12-C11	7.09	123.55	109.12
3	A	602	TCH	C6-C5-C4	7.07	119.30	111.23
3	A	602	TCH	C18-C13-C12	6.99	116.05	109.06
3	B	601	TCH	O3-C3-C4	6.66	123.10	109.84
3	B	602	TCH	C15-C14-C8	6.66	127.49	118.36
3	A	601	TCH	C13-C17-C20	6.64	127.52	119.48
3	A	601	TCH	C10-C9-C8	6.61	119.20	111.84
3	A	601	TCH	O12-C12-C11	6.52	122.39	109.12
3	A	602	TCH	O3-C3-C4	6.46	122.72	109.84
3	A	601	TCH	O3-C3-C4	6.45	122.68	109.84
3	B	601	TCH	C16-C17-C13	6.43	109.77	103.54
3	B	601	TCH	C18-C13-C12	6.22	115.28	109.06
3	A	601	TCH	C11-C12-C13	6.22	117.59	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TCH	C18-C13-C12	6.20	115.27	109.06
3	A	601	TCH	C15-C14-C8	6.20	126.86	118.36
3	A	602	TCH	C11-C12-C13	6.04	117.41	111.26
3	B	602	TCH	O3-C3-C4	5.99	121.76	109.84
3	B	602	TCH	C17-C13-C14	-5.93	94.17	100.11
3	B	601	TCH	C6-C5-C4	5.85	117.91	111.23
3	A	602	TCH	C16-C17-C13	5.77	109.13	103.54
3	A	602	TCH	C13-C17-C20	5.70	126.38	119.48
3	B	601	TCH	C5-C6-C7	-5.69	107.64	114.40
3	A	602	TCH	C17-C13-C14	-5.67	94.43	100.11
3	B	601	TCH	C15-C14-C8	5.60	126.04	118.36
3	A	601	TCH	C16-C17-C13	5.51	108.89	103.54
3	B	602	TCH	C6-C5-C4	5.46	117.46	111.23
3	B	602	TCH	C16-C17-C13	5.35	108.73	103.54
3	B	601	TCH	C13-C17-C20	5.33	125.94	119.48
3	B	601	TCH	C17-C13-C14	-5.30	94.80	100.11
3	B	601	TCH	C4-C3-C2	-5.24	104.22	110.62
3	B	602	TCH	C14-C8-C7	5.22	118.78	111.85
3	A	601	TCH	C17-C13-C14	-5.13	94.97	100.11
3	A	602	TCH	C15-C14-C8	5.09	125.33	118.36
3	B	601	TCH	C13-C14-C8	-5.01	108.37	114.72
3	B	602	TCH	C14-C8-C9	4.92	116.62	109.75
3	A	602	TCH	C4-C3-C2	-4.89	104.65	110.62
3	A	601	TCH	C4-C3-C2	-4.88	104.66	110.62
3	B	602	TCH	C11-C12-C13	4.74	116.09	111.26
3	B	601	TCH	O24-C24-N24	-4.71	113.78	123.03
3	A	601	TCH	O24-C24-N24	-4.70	113.81	123.03
3	A	601	TCH	C6-C5-C4	4.63	116.51	111.23
3	A	601	TCH	C14-C8-C7	4.58	117.93	111.85
3	A	602	TCH	C5-C4-C3	-4.54	105.85	112.71
3	B	601	TCH	C14-C8-C7	4.53	117.86	111.85
3	B	602	TCH	O24-C24-N24	-4.49	114.22	123.03
3	B	602	TCH	C13-C17-C20	4.46	124.89	119.48
3	A	601	TCH	C14-C8-C9	4.33	115.80	109.75
3	B	602	TCH	C9-C8-C7	-4.30	106.44	111.86
3	B	601	TCH	C18-C13-C14	-4.11	104.76	111.20
3	A	601	TCH	C13-C14-C8	-4.07	109.56	114.72
3	A	601	TCH	C14-C13-C12	-4.05	103.71	107.42
3	A	602	TCH	O24-C24-N24	-4.02	115.15	123.03
3	A	601	TCH	C18-C13-C14	-3.95	105.02	111.20
3	B	602	TCH	C4-C5-C10	-3.93	108.48	112.66
3	A	602	TCH	C14-C8-C9	3.83	115.10	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	TCH	C5-C4-C3	-3.79	107.00	112.71
3	B	602	TCH	C10-C9-C8	3.77	116.04	111.84
3	A	602	TCH	C18-C13-C14	-3.76	105.31	111.20
3	B	602	TCH	C16-C15-C14	-3.73	97.85	105.14
3	B	601	TCH	C26-C25-N24	3.71	122.37	111.41
3	A	602	TCH	C13-C14-C8	-3.65	110.10	114.72
3	B	602	TCH	C13-C14-C8	-3.62	110.14	114.72
3	B	602	TCH	C23-C22-C20	3.58	121.15	114.46
3	A	602	TCH	C21-C20-C17	-3.57	107.53	112.88
3	A	602	TCH	C16-C15-C14	-3.49	98.32	105.14
3	A	601	TCH	C26-C25-N24	3.41	121.49	111.41
3	B	601	TCH	C14-C8-C9	3.38	114.47	109.75
3	B	601	TCH	C23-C22-C20	3.31	120.65	114.46
3	B	602	TCH	C18-C13-C14	-3.28	106.07	111.20
3	B	602	TCH	C26-C25-N24	3.24	120.98	111.41
3	A	602	TCH	C26-C25-N24	3.17	120.77	111.41
3	B	602	TCH	C4-C3-C2	-3.16	106.76	110.62
3	A	601	TCH	C23-C22-C20	3.12	120.30	114.46
3	A	601	TCH	C16-C15-C14	-3.07	99.13	105.14
3	B	602	TCH	C6-C7-C8	3.06	114.84	111.50
3	A	601	TCH	C15-C16-C17	3.02	111.05	105.14
3	B	601	TCH	C16-C15-C14	-3.00	99.28	105.14
3	B	601	TCH	C15-C16-C17	2.99	110.99	105.14
3	A	601	TCH	O3-C3-C2	2.97	117.94	110.17
3	B	601	TCH	C21-C20-C17	-2.97	108.42	112.88
3	A	601	TCH	C5-C4-C3	-2.96	108.25	112.71
3	B	601	TCH	O3-C3-C2	2.95	117.88	110.17
3	A	602	TCH	C6-C5-C10	-2.89	109.59	112.66
3	A	601	TCH	C19-C10-C5	2.84	115.18	110.44
3	A	602	TCH	O3-C3-C2	2.82	117.54	110.17
3	A	602	TCH	C23-C22-C20	2.75	119.59	114.46
3	A	602	TCH	C1-C10-C9	-2.70	107.14	111.34
3	A	601	TCH	C22-C20-C17	2.70	115.93	110.33
3	A	601	TCH	C5-C6-C7	-2.69	111.21	114.40
3	B	602	TCH	C19-C10-C5	2.64	114.84	110.44
3	B	601	TCH	C6-C5-C10	-2.63	109.86	112.66
3	A	602	TCH	C19-C10-C5	2.63	114.83	110.44
3	A	602	TCH	C15-C16-C17	2.61	110.26	105.14
3	A	601	TCH	C4-C5-C10	-2.58	109.92	112.66
3	B	601	TCH	C19-C10-C5	2.54	114.69	110.44
3	B	602	TCH	C5-C4-C3	-2.54	108.88	112.71
2	B	600	NAG	C1-O5-C5	2.50	115.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	TCH	C21-C20-C17	-2.49	109.15	112.88
3	B	602	TCH	C15-C16-C17	2.48	109.99	105.14
3	A	602	TCH	C14-C8-C7	2.45	115.10	111.85
3	A	601	TCH	C19-C10-C9	-2.44	107.90	111.18
3	B	602	TCH	O1S-S26-C26	-2.44	103.05	106.73
3	A	601	TCH	O7-C7-C6	2.42	115.88	109.86
3	B	602	TCH	O3-C3-C2	2.41	116.47	110.17
3	B	602	TCH	C16-C17-C20	2.36	115.74	112.18
3	B	602	TCH	C9-C10-C5	-2.34	105.27	108.51
2	B	600	NAG	C8-C7-N2	-2.33	112.26	116.12
3	A	601	TCH	O1S-S26-C26	-2.32	103.22	106.73
3	B	602	TCH	O7-C7-C6	2.30	115.57	109.86
3	A	602	TCH	C6-C7-C8	2.28	113.99	111.50
2	A	600	NAG	C8-C7-N2	-2.25	112.38	116.12
3	A	601	TCH	C1-C2-C3	-2.24	107.52	110.48
3	A	602	TCH	C14-C13-C12	-2.23	105.38	107.42
3	B	601	TCH	O24-C24-C23	-2.19	118.05	122.02
3	B	601	TCH	C6-C7-C8	2.11	113.81	111.50
3	B	602	TCH	O24-C24-C23	-2.11	118.19	122.02
3	B	601	TCH	C22-C20-C17	2.08	114.65	110.33
2	A	600	NAG	C1-O5-C5	2.08	114.97	112.19
2	B	600	NAG	O7-C7-N2	2.06	125.62	121.98
3	A	602	TCH	C19-C10-C9	-2.04	108.43	111.18
3	A	601	TCH	O24-C24-C23	-2.04	118.32	122.02
3	B	601	TCH	O7-C7-C6	2.02	114.88	109.86
3	A	602	TCH	O24-C24-C23	-2.00	118.39	122.02

All (16) chirality outliers are listed below:

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

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

All (42) torsion outliers are listed below:

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

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

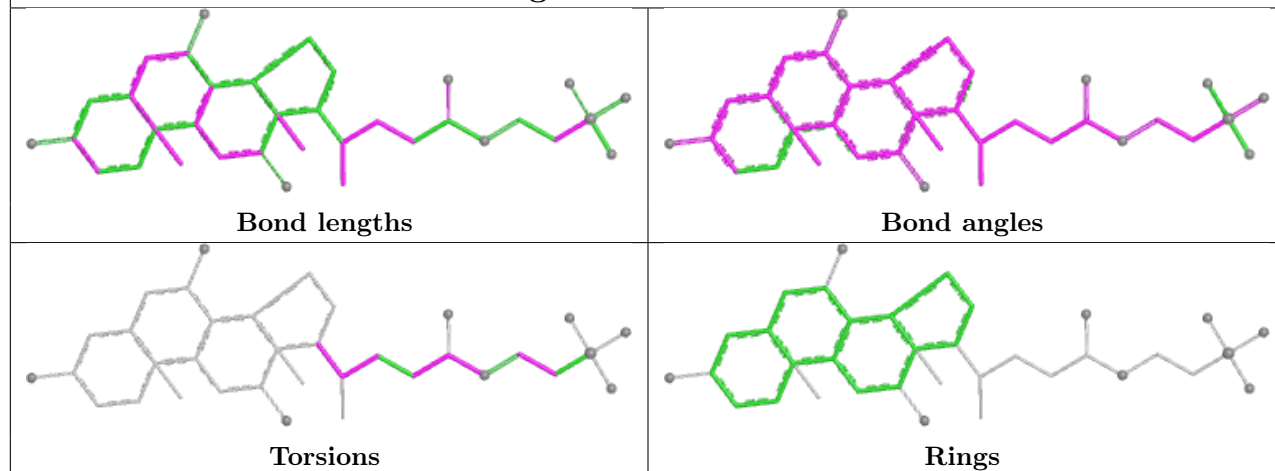
There are no ring outliers.

6 monomers are involved in 23 short contacts:

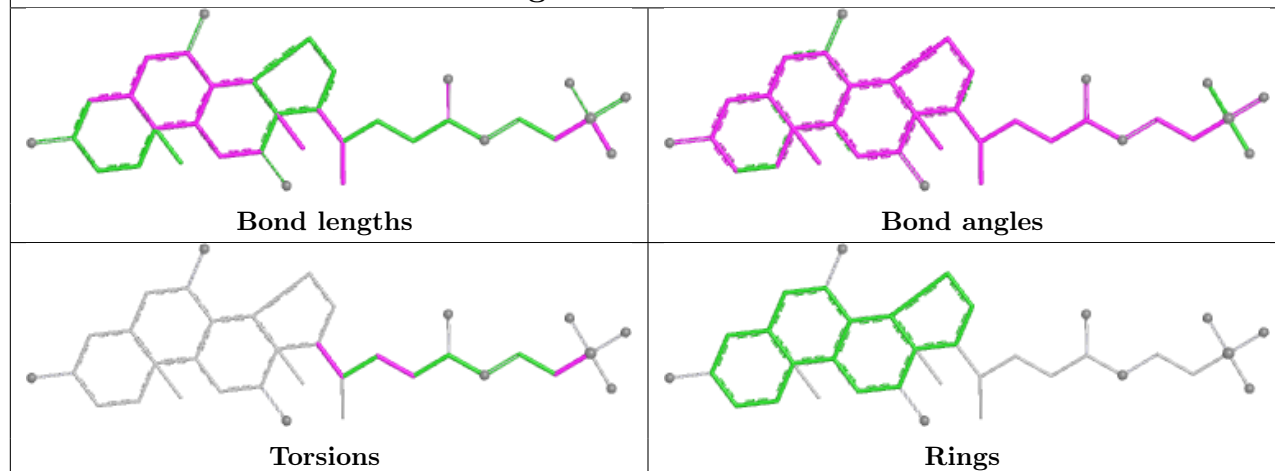
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	TCH	7	0
3	A	602	TCH	8	0
2	B	600	NAG	1	0
2	A	600	NAG	2	0
3	B	602	TCH	4	0
3	A	601	TCH	1	0

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 than 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.

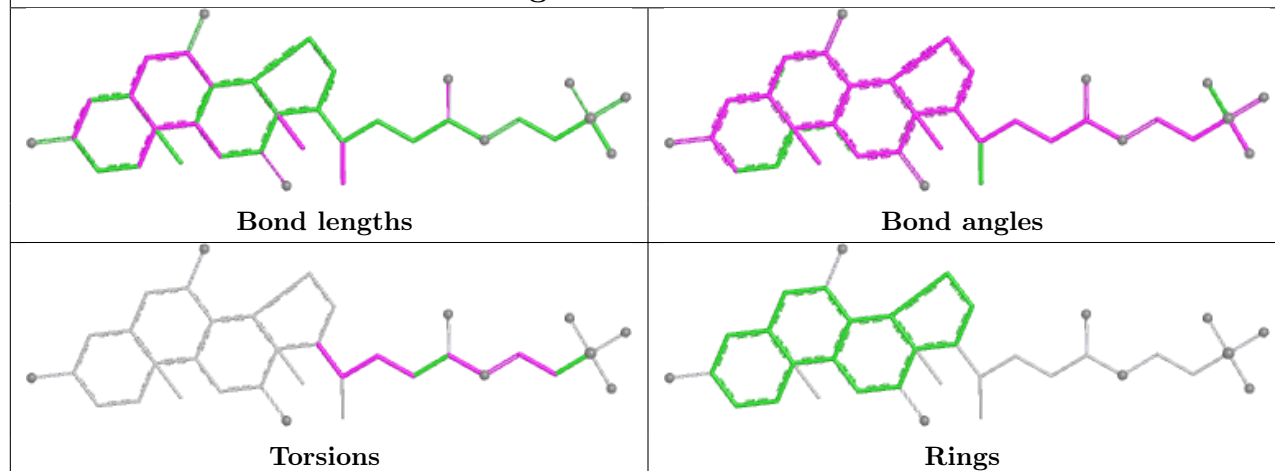
Ligand TCH B 601

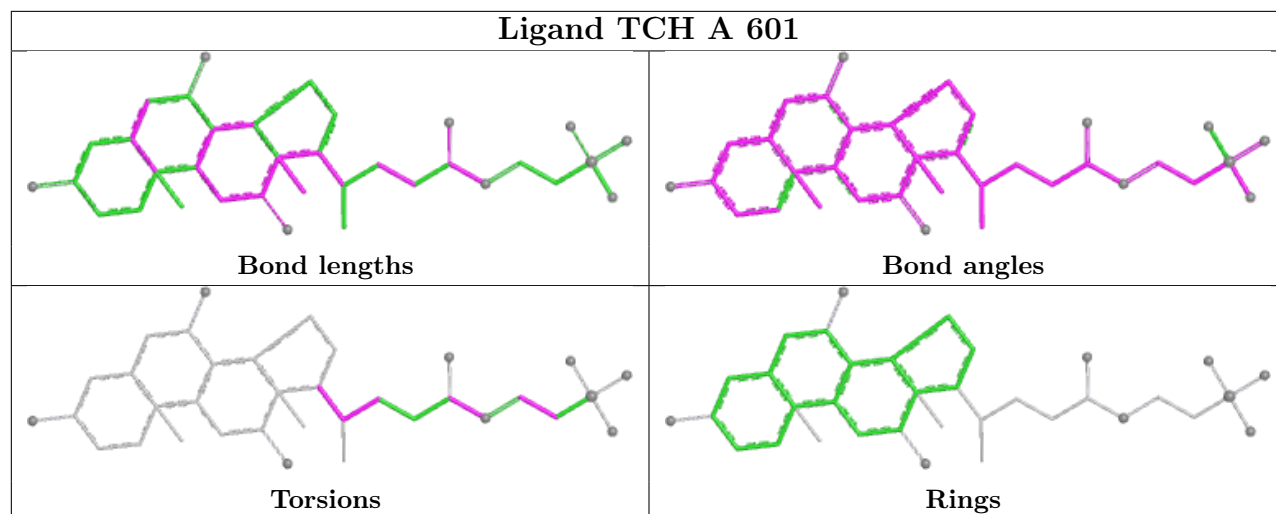


Ligand TCH A 602



Ligand TCH B 602





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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.