Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:13 am BST

PDB ID	:	2ISD
Title	:	PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM RAT
Authors	:	Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on	:	1997-03-31
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

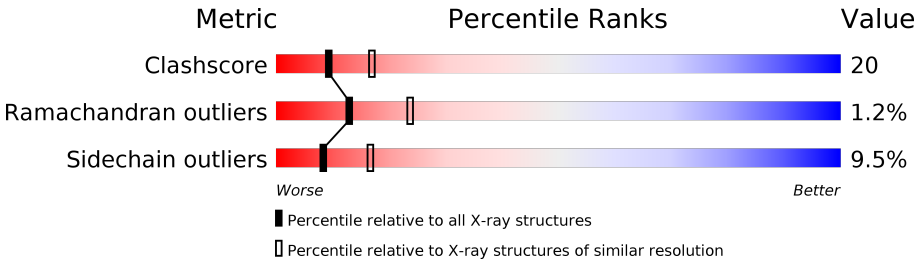
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	53% 27% • 18%
1	B	624	56% 30% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	5	-	-	X	-

2 Entry composition

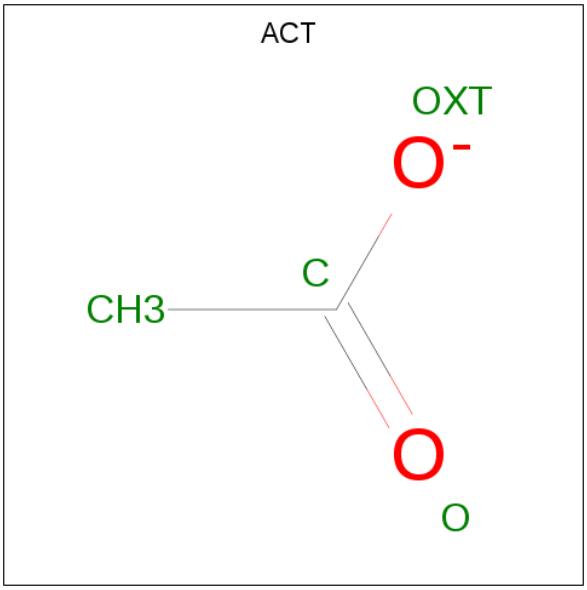
There are 3 unique types of molecules in this entry. The entry contains 9216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	106	0	0
			4070	2573	709	766	22			
1	B	561	Total	C	N	O	S	104	0	0
			4465	2818	776	847	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	316	Total O 316 316	0	0
3	B	357	Total O 357 357	0	0

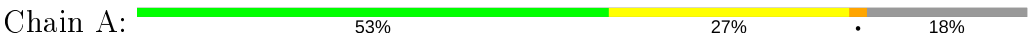
3 Residue-property plots (i)

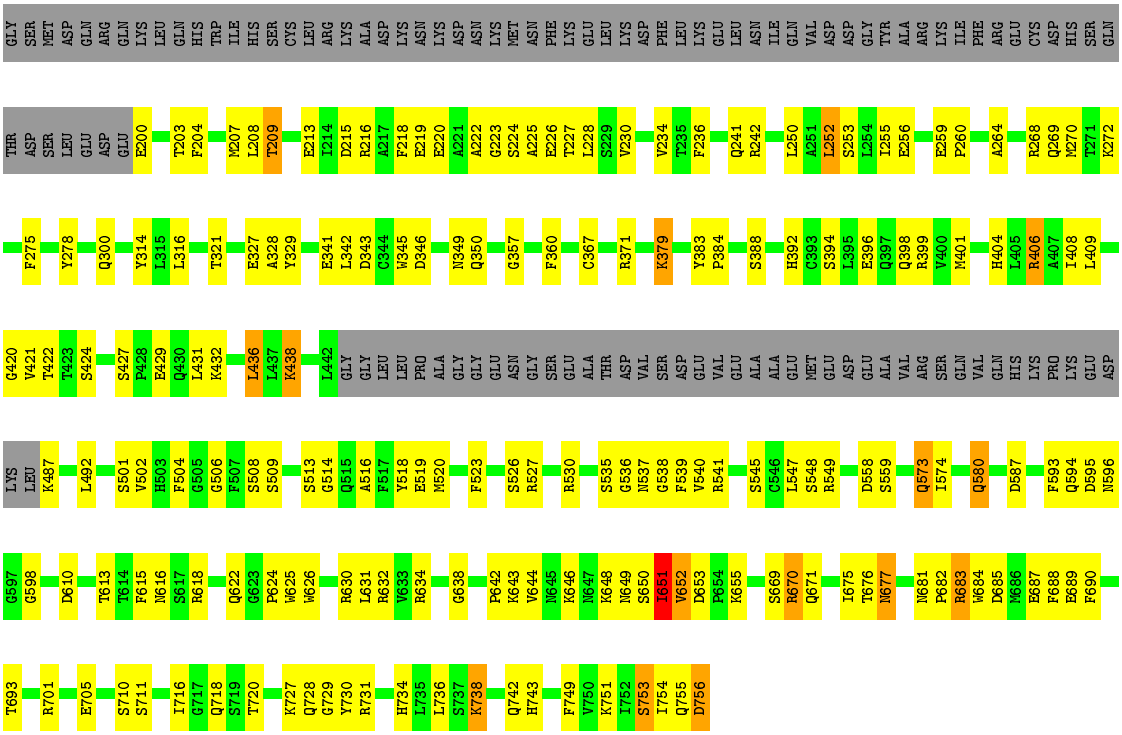
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1

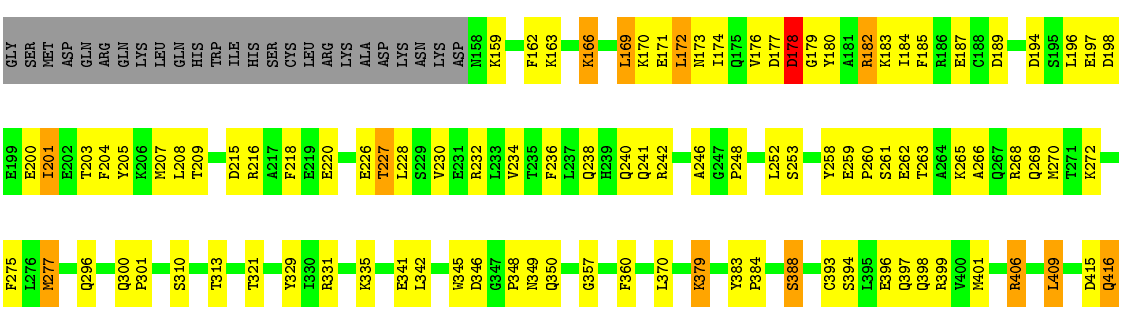
Chain A:

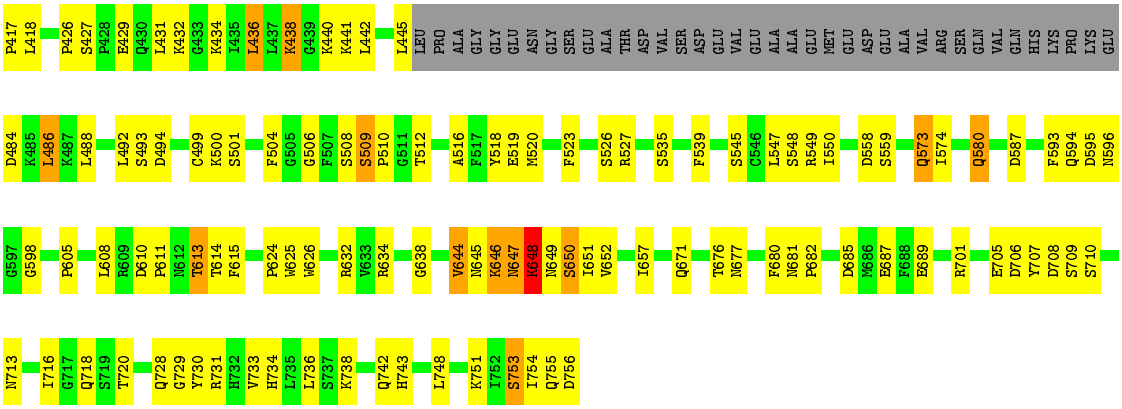




• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1

Chain B:




P417 L418 P426 S427 P428 E429 Q430 L431 K432 G433 K434 I435 L436 L437 K438 G439 K440 K441 L442 L445 LEU PRO ALA GLY GLY GLU ASN GLY SER GLU ALA THR ASP VAL SER ASP GLU VAL GLU ALA ALA GLU MET GLU ASP GLU ALA VAL ARG SER GLN VAL GLN HIS LYS PRO LYS GLU
D484 K485 L486 K487 L488 L492 S493 D494 C499 K500 S501 F504 G505 G506 F507 S508 S509 P510 G511 T512 A516 F517 Y518 E519 M520 F523 S526 R527 S535 F539 S545 C546 L547 S548 R549 I550 D558 S559 Q573 I574 Q580 D587 F593 Q594 D595 N596
G597 G598 P605 L608 R609 D610 P611 N612 T613 T614 F615 P624 W625 W626 R632 V633 R634 G638 V644 N645 K646 N647 K648 N649 S650 I651 V652 I657 Q671 T676 N677 F680 N681 P682 D685 M686 E687 F688 E689 R701 E705 D706 Y707 D708 S709 S710
N713 I716 G717 Q718 S719 T720 Q728 G729 Y730 R731 H732 V733 H734 L735 L736 S737 K738 Q742 H743 L748 K751 I752 S753 I754 Q755 D756

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	397.36Å 397.36Å 397.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.0 (15.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.227 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9216	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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: ACT

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	0.70	0/4165	0.79	3/5641 (0.1%)
1	B	0.69	0/4565	0.82	4/6174 (0.1%)
All	All	0.69	0/8730	0.81	7/11815 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	743	HIS	C-N-CD	-7.89	103.24	120.60
1	A	743	HIS	C-N-CD	-7.31	104.53	120.60
1	B	508	SER	N-CA-C	6.51	128.58	111.00
1	B	179	GLY	N-CA-C	-5.93	98.26	113.10
1	B	649	ASN	CB-CA-C	-5.46	99.47	110.40
1	A	420	GLY	N-CA-C	-5.21	100.09	113.10
1	A	514	GLY	N-CA-C	-5.02	100.56	113.10

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	4070	0	3994	145	0
1	B	4465	0	4375	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	316	0	0	13	2
3	B	357	0	0	13	1
All	All	9216	0	8375	326	2

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 20.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLY:N	3:A:1031:HOH:O	1.97	0.98
1:B:176:VAL:HG21	1:B:208:LEU:HD11	1.42	0.98
1:B:644:VAL:HG23	1:B:645:ASN:H	1.29	0.98
1:A:200:GLU:HA	1:A:203:THR:HB	1.45	0.96
1:B:573:GLN:H	1:B:573:GLN:HE21	1.15	0.94
1:B:486:LEU:H	1:B:486:LEU:HD12	1.34	0.93
1:A:573:GLN:H	1:A:573:GLN:HE21	1.05	0.93
1:A:573:GLN:H	1:A:573:GLN:NE2	1.70	0.90
1:B:171:GLU:HG3	1:B:172:LEU:HD13	1.56	0.88
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.55	0.88
1:B:573:GLN:H	1:B:573:GLN:NE2	1.73	0.86
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.57	0.84
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.60	0.84
1:B:176:VAL:HG21	1:B:208:LEU:CD1	2.07	0.84
1:A:241:GLN:HE22	1:A:730:TYR:H	1.22	0.83
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.61	0.82
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.61	0.82
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.61	0.81
1:A:651:ILE:HD12	1:A:677:ASN:ND2	1.97	0.80
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.65	0.79
1:B:234:VAL:O	1:B:238:GLN:HG3	1.83	0.78
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.13	0.78
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.66	0.77
1:B:241:GLN:HE22	1:B:730:TYR:H	1.33	0.76
1:B:728:GLN:NE2	1:B:754:ILE:H	1.84	0.76
1:B:429:GLU:OE1	1:B:432:LYS:HE2	1.86	0.76
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.21	0.76
1:A:252:LEU:O	1:A:256:GLU:HG3	1.87	0.75
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LYS:HA	3:B:908:HOH:O	1.86	0.73
1:B:436:LEU:N	1:B:436:LEU:HD23	2.04	0.73
1:B:196:LEU:HD22	1:B:200:GLU:CB	2.18	0.73
1:A:200:GLU:HA	1:A:203:THR:CB	2.18	0.72
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.71	0.71
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.20	0.70
1:B:178:ASP:HB3	1:B:180:TYR:H	1.57	0.69
1:A:436:LEU:N	1:A:436:LEU:HD23	2.06	0.69
1:A:520:MET:CE	1:A:549:ARG:HB2	2.22	0.69
1:B:203:THR:O	1:B:207:MET:HG3	1.93	0.69
1:A:613:THR:HG22	1:A:615:PHE:H	1.58	0.69
1:A:670:ARG:HD3	3:A:909:HOH:O	1.92	0.69
1:B:509:SER:N	1:B:510:PRO:HD2	2.07	0.69
1:B:227:THR:HG21	1:B:269:GLN:HB3	1.74	0.68
1:B:436:LEU:H	1:B:436:LEU:HD23	1.58	0.68
1:B:706:ASP:O	1:B:713:ASN:HB3	1.93	0.68
1:B:171:GLU:CG	1:B:172:LEU:HD13	2.23	0.68
1:B:646:LYS:HG3	1:B:647:ASN:N	2.08	0.68
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.74	0.68
1:B:708:ASP:HB2	3:B:1064:HOH:O	1.93	0.68
1:A:728:GLN:NE2	1:A:754:ILE:H	1.91	0.67
1:B:189:ASP:HB3	3:B:915:HOH:O	1.95	0.67
1:B:613:THR:HG22	1:B:615:PHE:H	1.60	0.66
1:A:573:GLN:NE2	1:A:573:GLN:N	2.44	0.65
1:A:730:TYR:CE1	1:A:751:LYS:HD2	2.31	0.65
1:A:630:ARG:NH1	3:A:886:HOH:O	2.29	0.65
1:A:755:GLN:HG2	1:A:756:ASP:N	2.11	0.65
1:B:176:VAL:HG23	1:B:680:PHE:CD2	2.31	0.65
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.32	0.65
1:B:174:ILE:HG23	1:B:176:VAL:HB	1.78	0.64
1:A:350:GLN:OE1	1:A:396:GLU:HG3	1.98	0.64
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.12	0.64
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.79	0.64
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.33	0.64
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.13	0.63
1:A:200:GLU:O	1:A:204:PHE:N	2.30	0.62
1:B:335:LYS:NZ	3:B:819:HOH:O	2.29	0.62
1:B:644:VAL:HG23	1:B:645:ASN:N	2.10	0.62
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.34	0.62
1:B:174:ILE:CG2	1:B:176:VAL:HB	2.30	0.62
1:B:205:TYR:O	1:B:209:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLU:CA	1:A:203:THR:HB	2.24	0.62
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.30	0.62
1:B:573:GLN:N	1:B:573:GLN:NE2	2.48	0.61
1:B:198:ASP:HA	1:B:201:ILE:HG13	1.83	0.61
1:A:651:ILE:HD12	1:A:677:ASN:HD21	1.64	0.61
1:A:379:LYS:HE2	3:A:916:HOH:O	2.00	0.60
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.83	0.60
1:B:171:GLU:O	1:B:172:LEU:HD22	2.01	0.60
1:B:172:LEU:O	1:B:174:ILE:HG13	2.01	0.60
1:B:196:LEU:O	1:B:201:ILE:HD11	2.01	0.60
1:A:215:ASP:OD1	1:A:272:LYS:NZ	2.30	0.60
1:A:429:GLU:OE1	1:A:432:LYS:HE2	2.01	0.60
1:A:632:ARG:HH22	1:B:406:ARG:CZ	2.15	0.60
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.37	0.59
1:A:203:THR:O	1:A:207:MET:N	2.30	0.59
1:B:520:MET:CE	1:B:549:ARG:HB2	2.33	0.59
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.37	0.59
1:B:440:LYS:HA	3:B:764:HOH:O	2.02	0.59
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.36	0.58
1:B:705:GLU:C	1:B:716:ILE:HD12	2.24	0.58
1:B:197:GLU:O	1:B:201:ILE:HG12	2.03	0.58
1:B:379:LYS:HE2	3:B:826:HOH:O	2.04	0.58
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.68	0.57
1:B:248:PRO:O	1:B:252:LEU:HB2	2.04	0.57
1:A:360:PHE:HE2	3:A:1013:HOH:O	1.87	0.57
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.36	0.57
1:B:520:MET:HE3	1:B:549:ARG:CB	2.34	0.57
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.51	0.57
1:B:728:GLN:HE21	1:B:753:SER:HA	1.70	0.57
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.87	0.56
1:A:343:ASP:HB3	3:A:821:HOH:O	2.04	0.56
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.40	0.56
1:B:216:ARG:O	1:B:220:GLU:HG3	2.05	0.56
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.36	0.56
1:A:736:LEU:HD23	1:A:742:GLN:HA	1.88	0.56
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.04	0.56
1:B:342:LEU:HD12	1:B:342:LEU:N	2.21	0.56
1:B:182:ARG:O	1:B:185:PHE:HB3	2.06	0.55
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.88	0.55
1:A:219:GLU:O	1:A:223:GLY:N	2.36	0.55
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASP:OD1	1:B:272:LYS:NZ	2.30	0.55
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.87	0.55
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.55
1:B:729:GLY:O	1:B:751:LYS:HA	2.07	0.55
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.19	0.55
1:A:573:GLN:HE21	1:A:573:GLN:N	1.89	0.55
1:B:548:SER:H	1:B:573:GLN:NE2	2.04	0.55
1:B:486:LEU:H	1:B:486:LEU:CD1	2.05	0.55
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.36	0.55
1:A:394:SER:O	1:A:398:GLN:HG3	2.07	0.54
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.08	0.54
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.08	0.54
1:B:348:PRO:HB2	1:B:349:ASN:HD22	1.73	0.54
1:A:241:GLN:HE22	1:A:730:TYR:N	2.01	0.54
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.37	0.54
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.72	0.54
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.08	0.53
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.34	0.53
1:B:595:ASP:OD1	1:B:596:ASN:N	2.40	0.53
1:B:593:PHE:O	1:B:598:GLY:HA2	2.07	0.53
1:A:218:PHE:CE1	1:A:272:LYS:HA	2.43	0.53
1:B:500:LYS:NZ	3:B:958:HOH:O	2.39	0.53
1:A:268:ARG:NE	3:A:904:HOH:O	2.30	0.53
1:B:163:LYS:HA	1:B:166:LYS:HB2	1.90	0.53
1:B:205:TYR:CE1	1:B:209:THR:HG21	2.44	0.53
1:B:218:PHE:CE1	1:B:272:LYS:HA	2.44	0.52
1:A:504:PHE:HB3	1:A:527:ARG:NH2	2.24	0.52
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.09	0.52
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.45	0.52
1:B:486:LEU:HD12	1:B:486:LEU:N	2.14	0.52
1:B:379:LYS:HE3	3:B:954:HOH:O	2.10	0.52
1:A:689:GLU:OE2	1:B:494:ASP:OD2	2.29	0.51
1:B:272:LYS:O	1:B:275:PHE:HB3	2.10	0.51
1:A:587:ASP:OD2	2:A:5:ACT:O	2.28	0.51
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.36	0.51
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.46	0.51
1:B:166:LYS:O	1:B:170:LYS:HG3	2.11	0.51
1:B:174:ILE:HG22	1:B:176:VAL:H	1.76	0.51
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.41	0.50
1:A:438:LYS:HE3	1:A:501:SER:OG	2.11	0.50
1:B:751:LYS:NZ	3:B:982:HOH:O	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.41	0.50
1:A:272:LYS:O	1:A:275:PHE:HB3	2.12	0.50
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.46	0.50
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.94	0.50
1:B:650:SER:HB3	3:B:868:HOH:O	2.11	0.50
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.59	0.50
1:B:227:THR:HG21	1:B:269:GLN:CD	2.31	0.50
1:A:227:THR:HG21	1:A:269:GLN:CD	2.32	0.50
1:A:230:VAL:O	1:A:234:VAL:HG23	2.12	0.50
1:B:730:TYR:C	1:B:731:ARG:HG2	2.31	0.50
1:A:593:PHE:O	1:A:598:GLY:HA2	2.11	0.49
1:A:558:ASP:O	1:A:559:SER:HB2	2.12	0.49
1:B:523:PHE:N	1:B:523:PHE:CD1	2.80	0.49
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.94	0.49
1:A:536:GLY:O	1:A:540:VAL:HG23	2.11	0.49
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.26	0.49
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.12	0.49
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.48	0.49
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.94	0.49
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.78	0.49
1:A:734:HIS:HE1	3:A:770:HOH:O	1.94	0.49
1:B:296:GLN:HA	3:B:907:HOH:O	2.13	0.49
1:A:651:ILE:HG22	1:A:677:ASN:C	2.33	0.49
1:A:350:GLN:HB3	3:A:1064:HOH:O	2.13	0.48
1:B:261:SER:O	1:B:265:LYS:HB2	2.13	0.48
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.02	0.48
1:A:729:GLY:O	1:A:751:LYS:HA	2.13	0.48
1:B:184:ILE:HG22	1:B:204:PHE:CD2	2.48	0.48
1:A:255:ILE:HD13	1:A:268:ARG:O	2.13	0.48
1:B:441:LYS:NZ	1:B:493:SER:O	2.47	0.48
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.28	0.48
1:A:523:PHE:CD1	1:A:523:PHE:N	2.81	0.48
1:A:634:ARG:NH2	1:A:751:LYS:HD3	2.28	0.48
1:B:174:ILE:HG22	1:B:176:VAL:HG12	1.96	0.48
1:A:349:ASN:O	1:A:350:GLN:HB2	2.13	0.48
1:B:177:ASP:O	1:B:178:ASP:HB2	2.14	0.48
1:A:264:ALA:O	1:A:269:GLN:N	2.46	0.48
1:B:701:ARG:NE	1:B:718:GLN:HE21	2.12	0.48
1:B:196:LEU:CD2	1:B:200:GLU:HB3	2.34	0.47
1:B:227:THR:CG2	1:B:228:LEU:N	2.77	0.47
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:LEU:CD2	1:B:742:GLN:HA	2.42	0.47
1:A:548:SER:H	1:A:573:GLN:NE2	2.13	0.47
1:B:183:LYS:O	1:B:187:GLU:HG3	2.14	0.47
1:B:258:TYR:HB3	1:B:277:MET:HB3	1.95	0.47
1:B:707:TYR:OH	1:B:709:SER:HB3	2.13	0.47
1:B:706:ASP:HB2	1:B:716:ILE:HD11	1.96	0.47
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.50	0.47
1:A:342:LEU:HD12	1:A:342:LEU:N	2.29	0.47
1:A:367:CYS:SG	1:A:371:ARG:NH2	2.87	0.47
1:B:259:GLU:OE1	1:B:270:MET:HA	2.14	0.47
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.45	0.47
1:A:436:LEU:H	1:A:436:LEU:HD23	1.78	0.47
1:A:648:LYS:O	1:A:650:SER:N	2.47	0.47
1:B:645:ASN:HB3	1:B:648:LYS:HD3	1.96	0.47
1:B:638:GLY:O	1:B:681:ASN:HA	2.15	0.46
1:A:644:VAL:HG12	1:A:644:VAL:O	2.14	0.46
1:A:705:GLU:C	1:A:716:ILE:HD12	2.36	0.46
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.97	0.46
1:B:426:PRO:HB2	1:B:431:LEU:HD11	1.97	0.46
1:B:398:GLN:OE1	1:B:488:LEU:HD12	2.16	0.46
1:B:580:GLN:HG2	3:B:810:HOH:O	2.15	0.46
1:B:647:ASN:HB2	1:B:648:LYS:H	1.46	0.46
1:B:509:SER:N	1:B:510:PRO:CD	2.78	0.46
1:B:313:THR:HB	1:B:329:TYR:CE1	2.51	0.46
1:A:222:ALA:HA	1:A:228:LEU:HD23	1.96	0.46
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.16	0.46
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.43	0.46
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.97	0.46
1:B:263:THR:O	1:B:266:ALA:HB3	2.16	0.46
1:B:734:HIS:HE1	3:B:828:HOH:O	1.99	0.46
1:A:349:ASN:O	1:A:349:ASN:OD1	2.33	0.46
1:B:625:TRP:CD1	1:B:626:TRP:N	2.84	0.46
1:B:169:LEU:O	1:B:171:GLU:O	2.34	0.45
1:B:227:THR:HG21	1:B:269:GLN:OE1	2.15	0.45
1:A:632:ARG:NH2	1:B:406:ARG:CZ	2.79	0.45
1:B:645:ASN:OD1	1:B:648:LYS:HD2	2.15	0.45
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.80	0.45
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.45
1:B:406:ARG:HH22	1:B:415:ASP:HB2	1.80	0.45
1:A:638:GLY:O	1:A:681:ASN:HA	2.16	0.45
1:A:653:ASP:OD1	1:A:677:ASN:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD11	1:B:431:LEU:CD2	2.46	0.45
1:B:632:ARG:NH1	1:B:689:GLU:OE1	2.50	0.45
1:A:626:TRP:CZ3	1:A:693:THR:HB	2.52	0.45
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.32	0.45
1:B:504:PHE:HB3	1:B:527:ARG:NH2	2.31	0.45
1:A:595:ASP:OD1	1:A:596:ASN:N	2.47	0.44
1:B:230:VAL:O	1:B:234:VAL:HG23	2.17	0.44
1:B:681:ASN:N	1:B:682:PRO:CD	2.80	0.44
1:B:406:ARG:HH11	1:B:406:ARG:CG	2.29	0.44
1:B:300:GLN:O	1:B:427:SER:HA	2.16	0.44
1:A:222:ALA:HA	1:A:228:LEU:CD2	2.47	0.44
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.79	0.44
1:B:227:THR:HG23	1:B:269:GLN:HB3	1.96	0.44
1:B:442:LEU:HD21	1:B:488:LEU:O	2.17	0.44
1:B:605:PRO:HD2	1:B:608:LEU:HD12	1.99	0.44
1:B:632:ARG:HH21	1:B:755:GLN:CD	2.20	0.44
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.33	0.44
1:B:644:VAL:CG2	1:B:645:ASN:H	2.10	0.44
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.51	0.44
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.47	0.44
1:A:259:GLU:OE1	1:A:270:MET:HA	2.17	0.44
1:A:670:ARG:HD3	3:A:850:HOH:O	2.17	0.44
1:B:394:SER:O	1:B:398:GLN:HG3	2.18	0.43
1:B:406:ARG:HH22	1:B:415:ASP:CB	2.30	0.43
1:B:610:ASP:O	1:B:613:THR:OG1	2.33	0.43
1:A:681:ASN:N	1:A:682:PRO:CD	2.80	0.43
1:B:396:GLU:O	1:B:399:ARG:HB2	2.18	0.43
1:A:730:TYR:C	1:A:731:ARG:HG2	2.38	0.43
1:B:198:ASP:O	1:B:201:ILE:HG13	2.19	0.43
1:A:341:GLU:C	1:A:342:LEU:HD12	2.39	0.43
1:B:657:ILE:HD13	1:B:671:GLN:HB3	2.01	0.43
1:A:631:LEU:O	1:A:689:GLU:HA	2.19	0.43
1:B:341:GLU:C	1:B:342:LEU:HD12	2.38	0.43
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.99	0.43
1:B:176:VAL:CG1	1:B:177:ASP:N	2.80	0.43
1:A:314:TYR:HB3	1:A:329:TYR:CE2	2.54	0.43
1:A:651:ILE:HB	1:A:677:ASN:ND2	2.33	0.43
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.99	0.42
1:A:396:GLU:O	1:A:399:ARG:HB2	2.19	0.42
1:A:710:SER:OG	1:A:711:SER:N	2.52	0.42
1:B:379:LYS:O	1:B:379:LYS:HG3	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:PRO:HG2	1:B:431:LEU:HD11	2.00	0.42
1:B:516:ALA:CB	1:B:518:TYR:CE2	3.00	0.42
1:B:558:ASP:O	1:B:559:SER:HB2	2.18	0.42
1:A:209:THR:HG22	1:A:209:THR:O	2.19	0.42
1:A:404:HIS:O	1:A:408:ILE:HG13	2.19	0.42
1:A:537:ASN:CA	3:A:1031:HOH:O	2.67	0.42
1:A:259:GLU:CD	1:A:260:PRO:HD2	2.39	0.42
1:A:218:PHE:CD1	1:A:272:LYS:HA	2.54	0.42
1:A:530:ARG:CZ	1:A:530:ARG:HB2	2.45	0.42
1:A:222:ALA:CB	1:A:228:LEU:HD23	2.50	0.42
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.87	0.42
1:B:549:ARG:O	1:B:550:ILE:HD13	2.19	0.42
1:B:580:GLN:HB2	1:B:580:GLN:HE21	1.47	0.42
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.49	0.42
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.55	0.42
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.54	0.42
1:A:738:LYS:HG2	2:A:5:ACT:H3	2.02	0.41
1:A:727:LYS:HE2	3:A:939:HOH:O	2.20	0.41
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.90	0.41
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.73	0.41
1:A:502:VAL:HG11	1:A:519:GLU:HB3	2.01	0.41
1:B:259:GLU:OE2	1:B:260:PRO:HD2	2.20	0.41
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.73	0.41
1:A:738:LYS:HE3	1:A:738:LYS:HB3	1.72	0.41
1:B:236:PHE:CD1	1:B:240:GLN:HG3	2.55	0.41
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.38	0.41
1:B:438:LYS:HE3	1:B:501:SER:OG	2.20	0.41
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.51	0.41
1:A:728:GLN:HE21	1:A:753:SER:HA	1.84	0.41
1:B:236:PHE:CE1	1:B:240:GLN:HG3	2.56	0.41
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.41	0.41
1:A:622:GLN:CA	1:B:445:LEU:CD1	2.99	0.41
1:B:610:ASP:HA	1:B:611:PRO:HD2	1.78	0.41
1:A:236:PHE:HA	3:A:866:HOH:O	2.19	0.41
1:A:687:GLU:HG2	1:A:688:PHE:N	2.36	0.41
1:B:436:LEU:N	1:B:436:LEU:CD2	2.79	0.41
1:A:300:GLN:O	1:A:427:SER:HA	2.20	0.41
1:A:516:ALA:CB	1:A:518:TYR:CZ	3.04	0.41
1:B:388:SER:OG	1:B:438:LYS:HD3	2.22	0.41
1:B:733:VAL:HB	1:B:748:LEU:HB2	2.02	0.41
1:A:537:ASN:O	1:A:541:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ARG:HG3	1:A:690:PHE:CE1	2.56	0.40
1:B:196:LEU:HD22	1:B:200:GLU:HB2	2.02	0.40
1:A:436:LEU:CD2	1:A:436:LEU:N	2.80	0.40
1:B:580:GLN:HG3	1:B:580:GLN:H	1.18	0.40
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.51	0.40
1:A:580:GLN:HG3	1:A:580:GLN:H	0.97	0.40
1:B:197:GLU:O	1:B:200:GLU:HB2	2.22	0.40
1:A:250:LEU:O	1:A:253:SER:OG	2.32	0.40
1:A:669:SER:C	1:A:670:ARG:HG2	2.42	0.40
1:B:370:LEU:HA	1:B:370:LEU:HD23	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:889:HOH:O	3:A:889:HOH:O[52_555]	2.00	0.20
3:A:990:HOH:O	3:B:966:HOH:O[24_555]	2.19	0.01

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	509/624 (82%)	468 (92%)	34 (7%)	7 (1%)	11	20
1	B	557/624 (89%)	509 (91%)	42 (8%)	6 (1%)	14	26
All	All	1066/1248 (85%)	977 (92%)	76 (7%)	13 (1%)	13	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	646	LYS
1	B	178	ASP

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Mol	Chain	Res	Type
1	B	647	ASN
1	A	209	THR
1	A	649	ASN
1	A	651	ILE
1	B	173	ASN
1	B	648	LYS
1	B	644	VAL
1	A	225	ALA
1	A	421	VAL
1	B	512	THR
1	A	652	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	448/545 (82%)	410 (92%)	38 (8%)	10 21
1	B	492/545 (90%)	441 (90%)	51 (10%)	7 13
All	All	940/1090 (86%)	851 (90%)	89 (10%)	8 17

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	220	GLU
1	A	224	SER
1	A	226	GLU
1	A	242	ARG
1	A	252	LEU
1	A	278	TYR
1	A	379	LYS
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	422	THR

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Mol	Chain	Res	Type
1	A	424	SER
1	A	436	LEU
1	A	438	LYS
1	A	487	LYS
1	A	508	SER
1	A	509	SER
1	A	513	SER
1	A	526	SER
1	A	535	SER
1	A	539	PHE
1	A	545	SER
1	A	573	GLN
1	A	574	ILE
1	A	580	GLN
1	A	594	GLN
1	A	643	LYS
1	A	651	ILE
1	A	652	VAL
1	A	670	ARG
1	A	676	THR
1	A	677	ASN
1	A	683	ARG
1	A	685	ASP
1	A	738	LYS
1	A	753	SER
1	A	756	ASP
1	B	159	LYS
1	B	166	LYS
1	B	169	LEU
1	B	172	LEU
1	B	178	ASP
1	B	182	ARG
1	B	194	ASP
1	B	201	ILE
1	B	226	GLU
1	B	227	THR
1	B	232	ARG
1	B	242	ARG
1	B	253	SER
1	B	262	GLU
1	B	268	ARG
1	B	277	MET

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Mol	Chain	Res	Type
1	B	310	SER
1	B	331	ARG
1	B	379	LYS
1	B	388	SER
1	B	406	ARG
1	B	409	LEU
1	B	416	GLN
1	B	436	LEU
1	B	438	LYS
1	B	484	ASP
1	B	486	LEU
1	B	499	CYS
1	B	509	SER
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	545	SER
1	B	573	GLN
1	B	574	ILE
1	B	580	GLN
1	B	594	GLN
1	B	613	THR
1	B	614	THR
1	B	646	LYS
1	B	648	LYS
1	B	650	SER
1	B	651	ILE
1	B	652	VAL
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	710	SER
1	B	738	LYS
1	B	753	SER
1	B	756	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	312	ASN
1	A	573	GLN

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Mol	Chain	Res	Type
1	A	580	GLN
1	A	594	GLN
1	A	639	GLN
1	A	677	ASN
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	A	743	HIS
1	B	210	GLN
1	B	241	GLN
1	B	312	ASN
1	B	349	ASN
1	B	573	GLN
1	B	594	GLN
1	B	639	GLN
1	B	677	ASN
1	B	718	GLN
1	B	728	GLN
1	B	734	HIS
1	B	743	HIS

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

2 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	ACT	B	5	-	1,3,3	3.67	1 (100%)	0,3,3	0.00	-
2	ACT	A	5	-	1,3,3	3.75	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	ACT	CH3-C	3.75	1.53	1.48
2	B	5	ACT	CH3-C	3.67	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	ACT	2	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 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.