



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 PM UTC

PDB ID : 2ISD / pdb_00002isd
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 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
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

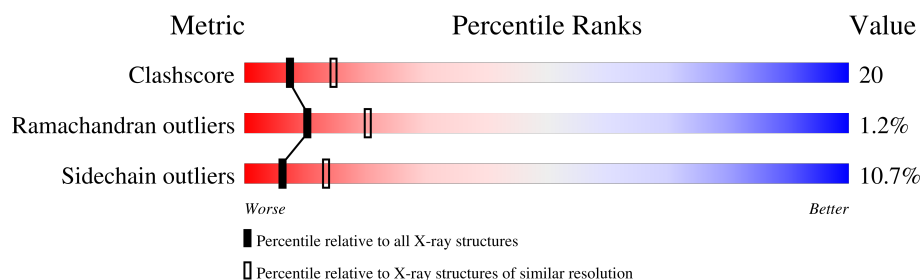
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	624	
1	B	624	

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 [i](#)

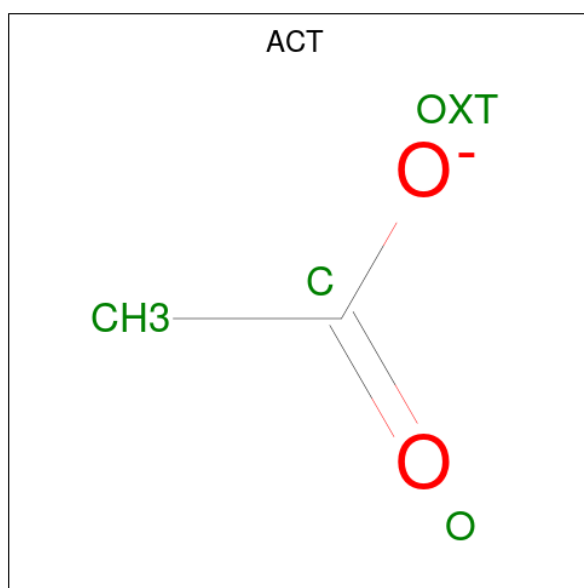
There are 3 unique types of molecules in this entry. The entry contains 9216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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.

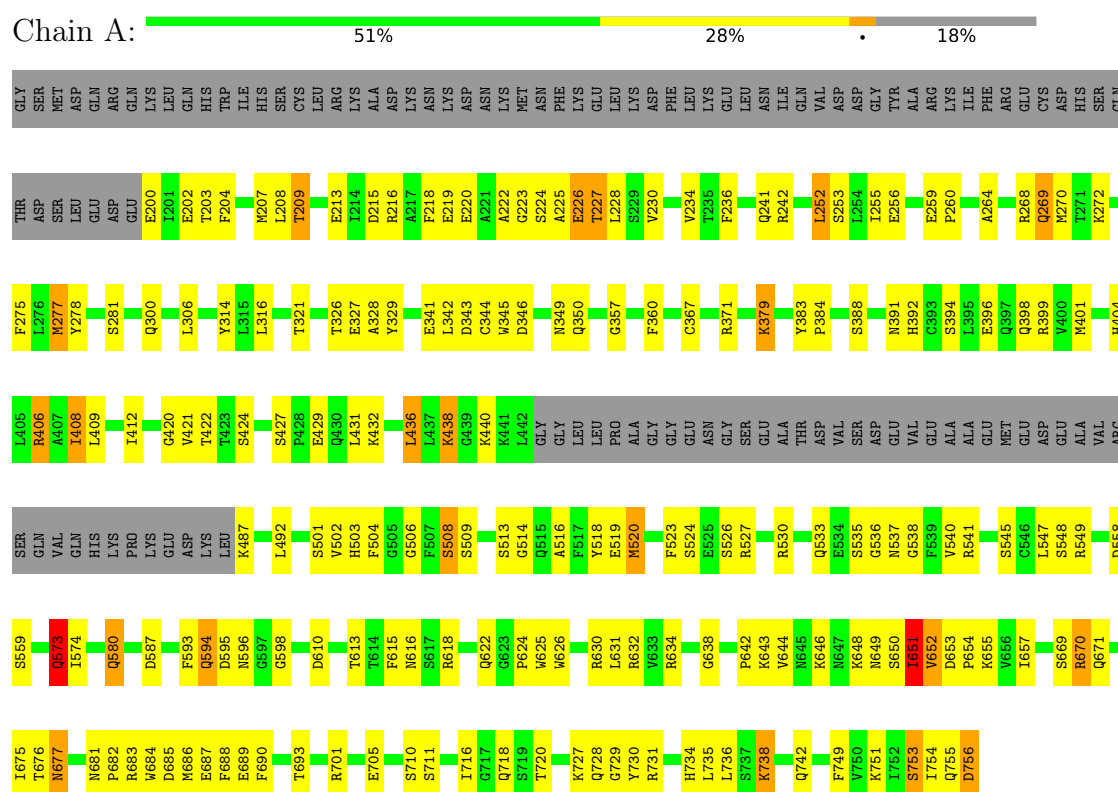
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	316	Total 316	O 316	0	0
3	B	357	Total 357	O 357	0	0

3 Residue-property plots

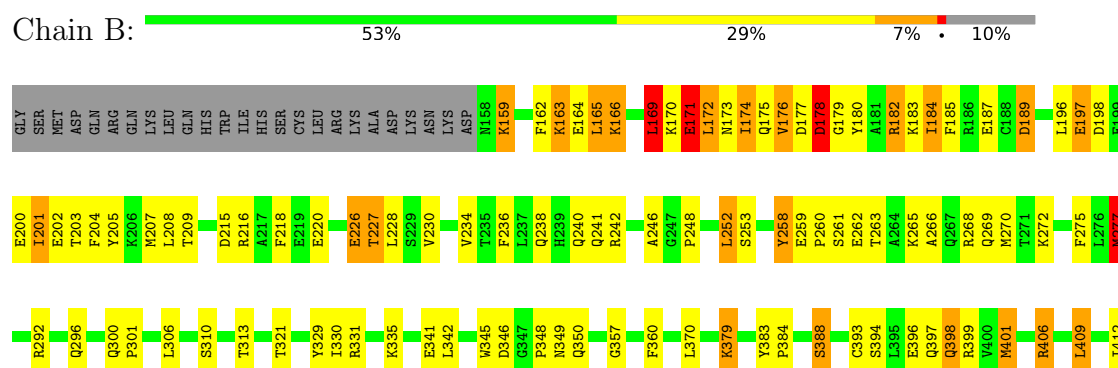
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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





4 Data and refinement statistics

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	397.36 Å 397.36 Å 397.36 Å 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	0.91	2/4165 (0.0%)	1.10	17/5641 (0.3%)
1	B	0.92	5/4565 (0.1%)	1.17	32/6174 (0.5%)
All	All	0.92	7/8730 (0.1%)	1.14	49/11815 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	520	MET	SD-CE	-8.96	1.57	1.79
1	A	277	MET	SD-CE	5.99	1.94	1.79
1	B	649	ASN	CA-C	-5.66	1.45	1.52
1	B	401	MET	SD-CE	-5.42	1.66	1.79
1	B	277	MET	SD-CE	5.31	1.92	1.79
1	B	330	ILE	CA-CB	-5.21	1.48	1.54
1	A	520	MET	SD-CE	-5.18	1.66	1.79

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	GLY	N-CA-C	-13.22	98.26	114.66
1	B	508	SER	N-CA-C	12.73	128.58	113.18
1	A	508	SER	N-CA-C	8.82	123.87	113.20
1	A	202	GLU	N-CA-C	-8.00	101.33	112.45
1	B	306	LEU	N-CA-C	-7.15	97.95	109.96
1	A	226	GLU	N-CA-C	-7.10	104.36	113.16
1	B	226	GLU	N-CA-C	-7.02	104.32	113.17
1	B	594	GLN	N-CA-C	-7.02	104.52	113.23
1	B	176	VAL	N-CA-C	-6.84	104.11	113.00
1	B	175	GLN	N-CA-C	-6.69	103.43	112.26
1	A	344	CYS	N-CA-C	6.44	120.15	109.46
1	B	164	GLU	N-CA-C	-6.39	104.36	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	LEU	N-CA-C	-6.34	99.31	109.96
1	B	171	GLU	N-CA-C	-6.25	100.58	109.96
1	B	591	GLY	N-CA-C	-6.23	104.95	112.49
1	B	654	PRO	N-CA-C	6.20	121.23	111.38
1	B	159	LYS	N-CA-C	-6.16	99.60	108.60
1	B	258	TYR	N-CA-C	6.05	121.33	113.88
1	A	594	GLN	N-CA-C	-6.05	105.39	112.89
1	B	649	ASN	CB-CA-C	-6.03	99.47	110.63
1	B	650	SER	N-CA-C	6.00	117.79	110.41
1	B	651	ILE	N-CA-C	-5.87	99.97	108.89
1	B	202	GLU	N-CA-C	-5.86	104.58	110.97
1	B	608	LEU	N-CA-C	-5.76	106.16	112.72
1	B	614	THR	N-CA-C	-5.73	105.95	113.17
1	A	326	THR	N-CA-C	-5.69	105.17	111.71
1	B	497	ILE	N-CA-C	5.68	116.82	111.48
1	B	712	LYS	N-CA-C	-5.63	102.15	110.48
1	B	165	LEU	N-CA-C	-5.61	104.80	111.03
1	A	735	LEU	N-CA-C	5.61	118.58	110.28
1	A	420	GLY	N-CA-C	-5.52	100.09	113.18
1	A	269	GLN	N-CA-C	5.52	118.59	110.59
1	A	654	PRO	N-CA-C	5.51	120.14	111.38
1	B	169	LEU	N-CA-C	-5.49	105.20	111.07
1	B	520	MET	N-CA-C	5.46	117.31	108.41
1	A	408	ILE	N-CA-C	5.45	116.11	110.82
1	A	524	SER	N-CA-C	-5.39	103.78	110.41
1	A	514	GLY	N-CA-C	-5.33	100.56	113.18
1	B	743	HIS	C-N-CD	-5.31	103.24	125.00
1	B	197	GLU	N-CA-C	-5.30	103.53	110.53
1	A	573	GLN	N-CA-C	5.26	119.70	113.12
1	B	615	PHE	N-CA-C	5.22	117.79	110.23
1	B	398	GLN	N-CA-C	-5.21	105.60	111.28
1	B	524	SER	N-CA-C	-5.21	103.66	110.53
1	B	560	SER	N-CA-C	-5.20	104.01	110.41
1	B	189	ASP	N-CA-C	5.20	117.14	107.99
1	A	391	ASN	N-CA-C	5.10	117.07	108.96
1	B	174	ILE	N-CA-C	5.04	115.29	107.78
1	A	503	HIS	N-CA-C	-5.02	103.05	110.48

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	149	0
1	B	4465	0	4375	194	0
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	316	0	0	14	2
3	B	357	0	0	13	1
All	All	9216	0	8375	333	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 (333) 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:520:MET:HE3	1:A:549:ARG:HB2	1.46	0.97
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:A:401:MET:HE2	1:A:492:LEU:HD11	1.55	0.88
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: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:B:520:MET:HE3	1:B:549:ARG:HB2	1.63	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:401:MET:HE2	1:B:492:LEU:HD11	1.71	0.72
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:HE3	1:A:549:ARG:CB	2.21	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:HD23	1:B:436:LEU:H	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:A:520:MET:CE	1:A:549:ARG:HB2	2.22	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:335:LYS:NZ	3:B:819:HOH:O	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:705:GLU:C	1:B:716:ILE:HD12	2.24	0.61
1:B:573:GLN:NE2	1:B:573:GLN:N	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:751:LYS:NZ	3:B:982:HOH:O	2.35	0.58
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:O	1:B:220:GLU:HG3	2.05	0.56
1:B:520:MET:HE3	1:B:549:ARG:CB	2.34	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
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:227:THR:HG21	1:B:269:GLN:CD	2.31	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:HA	1:A:327:GLU:OE1	2.08	0.54
1:B:730:TYR:C	1:B:731:ARG:HG2	2.31	0.54
1:A:227:THR:HG21	1:A:269:GLN:CD	2.32	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:HH11	1:A:216:ARG:HG3	1.72	0.54
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.08	0.53
1:A:651:ILE:HG22	1:A:677:ASN:C	2.33	0.53
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.34	0.53
1:B:593:PHE:O	1:B:598:GLY:HA2	2.07	0.53
1:B:595:ASP:OD1	1:B:596:ASN:N	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:705:GLU:C	1:A:716:ILE:HD12	2.36	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: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:A:230:VAL:O	1:A:234:VAL:HG23	2.12	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:HG3	1:A:216:ARG:NH1	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:632:ARG:HH21	1:B:755:GLN:CD	2.20	0.49
1:B:296:GLN:HA	3:B:907:HOH:O	2.13	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:B:341:GLU:C	1:B:342:LEU:HD12	2.38	0.48
1:A:255:ILE:HD13	1:A:268:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:523:PHE:CD1	2.81	0.48
1:A:634:ARG:NH2	1:A:751:LYS:HD3	2.28	0.48
1:A:730:TYR:C	1:A:731:ARG:HG2	2.38	0.48
1:B:174:ILE:HG22	1:B:176:VAL:HG12	1.96	0.48
1:A:341:GLU:C	1:A:342:LEU:HD12	2.39	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
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:A:259:GLU:CD	1:A:260:PRO:HD2	2.39	0.47
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.45	0.47
1:A:436:LEU:HD23	1:A:436:LEU:H	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:B:610:ASP:O	1:B:613:THR:OG1	2.33	0.46
1:A:644:VAL:HG12	1:A:644:VAL:O	2.14	0.46
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.97	0.46
1:A:686:MET:HE3	1:A:687:GLU:O	2.15	0.46
1:B:398:GLN:OE1	1:B:488:LEU:HD12	2.16	0.46
1:B:426:PRO:HB2	1:B:431:LEU:HD11	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.16	0.46
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.97	0.46
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.43	0.46
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.41	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: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
1:A:278:TYR:O	1:A:281:SER:OG	2.30	0.45
1:A:669:SER:C	1:A:670:ARG:HG2	2.42	0.45
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:227:THR:CG2	1:A:228:LEU:N	2.79	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:300:GLN:O	1:B:427:SER:HA	2.16	0.44
1:B:406:ARG:HH11	1:B:406:ARG:CG	2.29	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: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:B:549:ARG:C	1:B:550:ILE:HD13	2.43	0.44
1:A:670:ARG:HD3	3:A:850:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:198:ASP:O	1:B:201:ILE:HG13	2.19	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:A:316:LEU:HD23	1:A:328:ALA:HB2	1.99	0.43
1:B:329:TYR:OH	1:B:341:GLU:O	2.36	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
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:O	1:A:209:THR:HG22	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: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:HD23	1:B:196:LEU:HA	1.87	0.42
1:B:549:ARG:O	1:B:550:ILE:HD13	2.19	0.42
1:B:580:GLN:HE21	1:B:580:GLN:HB2	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:401:MET:HE2	1:A:492:LEU:CD1	2.37	0.41
1:A:727:LYS:HE2	3:A:939:HOH:O	2.20	0.41
1:B:434:LYS:HA	1:B:434:LYS:HD2	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:A:537:ASN:C	3:A:1031:HOH:O	2.51	0.41
1:B:259:GLU:OE2	1:B:260:PRO:HD2	2.20	0.41
1:B:409:LEU:HA	1:B:409:LEU:HD12	1.73	0.41
1:A:738:LYS:HB3	1:A:738:LYS:HE3	1.72	0.41
1:B:236:PHE:CD1	1:B:240:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:622:GLN:CA	1:B:445:LEU:CD1	2.99	0.41
1:B:292:ARG:C	1:B:597:GLY:HA2	2.45	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
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:N	1:A:436:LEU:CD2	2.80	0.40
1:B:204:PHE:CD1	1:B:204:PHE:C	2.99	0.40
1:B:580:GLN:H	1:B:580:GLN:HG3	1.18	0.40
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.51	0.40
1:A:580:GLN:H	1:A:580:GLN:HG3	0.97	0.40
1:B:197:GLU:O	1:B:200:GLU:HB2	2.22	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%)	9	17
1	B	557/624 (89%)	509 (91%)	42 (8%)	6 (1%)	11	22
All	All	1066/1248 (85%)	977 (92%)	76 (7%)	13 (1%)	10	20

All (13) Ramachandran outliers are listed below:

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

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%)	406 (91%)	42 (9%)	8	18
1	B	492/545 (90%)	433 (88%)	59 (12%)	5	10
All	All	940/1090 (86%)	839 (89%)	101 (11%)	6	13

All (101) 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	227	THR
1	A	242	ARG
1	A	252	LEU
1	A	253	SER
1	A	277	MET
1	A	379	LYS
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	412	ILE
1	A	422	THR
1	A	424	SER
1	A	436	LEU
1	A	438	LYS
1	A	440	LYS
1	A	487	LYS
1	A	508	SER
1	A	509	SER
1	A	513	SER
1	A	526	SER
1	A	533	GLN
1	A	535	SER
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	657	ILE
1	A	670	ARG
1	A	676	THR
1	A	677	ASN
1	A	685	ASP
1	A	738	LYS
1	A	753	SER
1	A	756	ASP
1	B	159	LYS

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Mol	Chain	Res	Type
1	B	163	LYS
1	B	165	LEU
1	B	166	LYS
1	B	169	LEU
1	B	171	GLU
1	B	172	LEU
1	B	178	ASP
1	B	182	ARG
1	B	184	ILE
1	B	201	ILE
1	B	226	GLU
1	B	227	THR
1	B	242	ARG
1	B	252	LEU
1	B	253	SER
1	B	262	GLU
1	B	268	ARG
1	B	277	MET
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	412	ILE
1	B	416	GLN
1	B	436	LEU
1	B	438	LYS
1	B	441	LYS
1	B	484	ASP
1	B	486	LEU
1	B	489	VAL
1	B	499	CYS
1	B	508	SER
1	B	509	SER
1	B	526	SER
1	B	535	SER
1	B	545	SER
1	B	573	GLN
1	B	574	ILE
1	B	577	LEU
1	B	580	GLN

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Mol	Chain	Res	Type
1	B	613	THR
1	B	614	THR
1	B	643	LYS
1	B	646	LYS
1	B	648	LYS
1	B	650	SER
1	B	651	ILE
1	B	652	VAL
1	B	657	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	312	ASN
1	A	515	GLN
1	A	573	GLN
1	A	580	GLN
1	A	594	GLN
1	A	677	ASN
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	A	743	HIS
1	B	190	HIS
1	B	210	GLN
1	B	238	GLN
1	B	241	GLN
1	B	304	HIS
1	B	312	ASN
1	B	349	ASN
1	B	573	GLN
1	B	580	GLN
1	B	594	GLN
1	B	677	ASN

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Mol	Chain	Res	Type
1	B	718	GLN
1	B	728	GLN
1	B	734	HIS
1	B	743	HIS

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](#)

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	A	5	-	3,3,3	0.97	0	3,3,3	0.92	0
2	ACT	B	5	-	3,3,3	1.01	0	3,3,3	0.64	0

There are no bond length outliers.

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.