WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 12:10 AM EST

PDB ID	:	1QAS
Title	:	1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-ESTERASE DELTA 1
Authors	:	Grobler, J.A.; Hurley, J.H.
Deposited on	:	1996-08-02
Resolution	:	2.40 Å(reported)

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

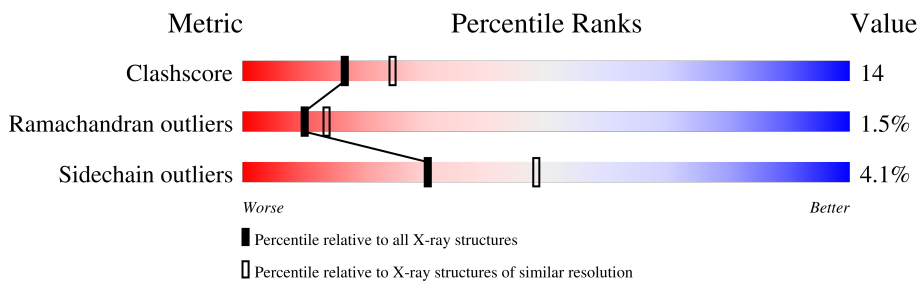|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		1.5%
Sidechain outliers		4.1%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	55% 23% • 19%
1	B	622	56% 23% • 19%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8235 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 PHOSPHOLIPASE C DELTA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3990	2522	696	750	22			
1	B	504	Total	C	N	O	S	0	0	0
			3979	2517	696	744	22			

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	134	Total	O	0	0
			134	134		

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.
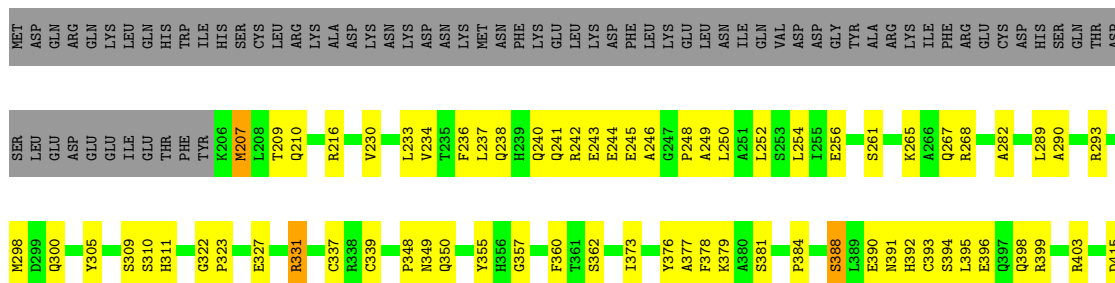
Note EDS was not executed.

• Molecule 1: PHOSPHOLIPASE C DELTA-1
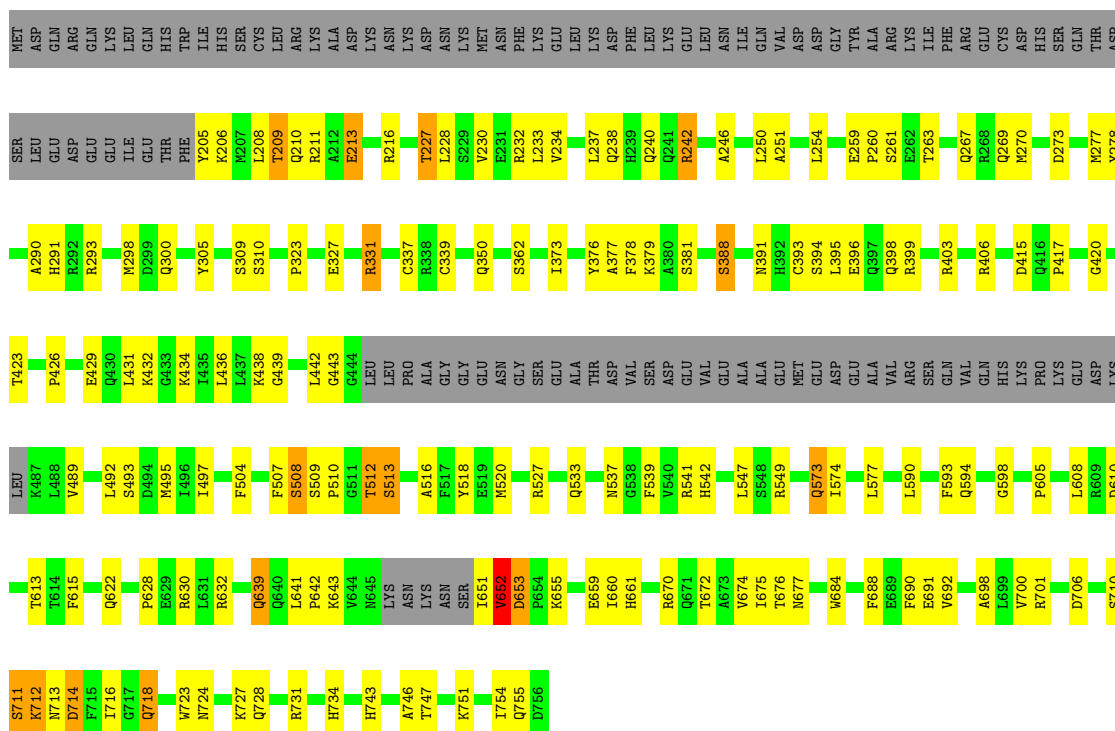
• Molecule 1: PHOSPHOLIPASE C DELTA-1
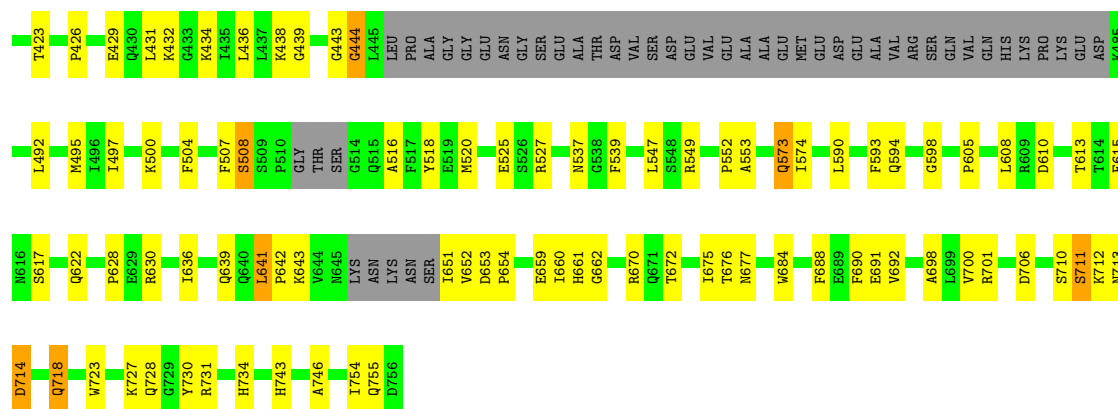
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.10Å 75.40Å 86.90Å 66.90° 85.40° 89.80°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8235	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.51	0/4083	0.79	5/5531 (0.1%)
1	B	0.52	0/4070	0.78	5/5511 (0.1%)
All	All	0.51	0/8153	0.78	10/11042 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	331	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	B	331	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	B	331	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	331	ARG	CD-NE-CZ	7.38	133.93	123.60
1	B	331	ARG	CD-NE-CZ	6.68	132.95	123.60
1	A	443	GLY	N-CA-C	-6.45	96.98	113.10
1	B	207	MET	CG-SD-CE	6.15	110.04	100.20
1	B	244	GLU	N-CA-C	-5.71	95.58	111.00
1	A	577	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3990	0	3906	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3979	0	3903	109	0
2	A	132	0	0	5	0
2	B	134	0	0	7	0
All	All	8235	0	7809	222	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 14.

All (222) 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:520:MET:HE3	1:A:549:ARG:HB2	1.47	0.95
1:A:228:LEU:HB2	1:A:270:MET:HB3	1.47	0.94
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.60	0.82
1:A:399:ARG:O	1:A:403:ARG:HG2	1.79	0.82
1:A:573:GLN:H	1:A:573:GLN:HE21	1.31	0.79
1:B:399:ARG:O	1:B:403:ARG:HG2	1.82	0.79
1:B:438:LYS:HE3	1:B:520:MET:HE1	1.66	0.78
1:B:241:GLN:HE22	1:B:730:TYR:H	1.31	0.77
1:B:734:HIS:HE1	2:B:2534:HOH:O	1.68	0.76
1:B:282:ALA:HB1	1:B:289:LEU:HD13	1.66	0.76
1:B:207:MET:HA	1:B:210:GLN:NE2	2.00	0.75
1:A:590:LEU:O	1:A:594:GLN:HG2	1.87	0.74
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.70	0.74
1:B:246:ALA:HB3	1:B:250:LEU:HB2	1.71	0.73
1:B:339:CYS:HB3	2:B:2946:HOH:O	1.89	0.72
1:B:323:PRO:HA	1:B:362:SER:HB3	1.73	0.70
1:A:701:ARG:HE	1:A:718:GLN:HE21	1.38	0.69
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.23	0.69
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.38	0.69
1:B:391:ASN:HD21	1:B:393:CYS:HB2	1.58	0.68
1:B:309:SER:OG	1:B:574:ILE:HG23	1.93	0.68
1:B:507:PHE:O	1:B:508:SER:HB2	1.94	0.68
1:B:573:GLN:H	1:B:573:GLN:HE21	1.42	0.68
1:A:339:CYS:HB3	2:A:2235:HOH:O	1.94	0.68
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.76	0.67
1:A:439:GLY:HA2	2:A:2318:HOH:O	1.94	0.67
1:B:298:MET:HB2	1:B:429:GLU:HG2	1.76	0.66
1:B:590:LEU:O	1:B:594:GLN:HG2	1.96	0.66
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.78	0.66
1:A:395:LEU:HD22	1:A:489:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLN:H	1:A:573:GLN:NE2	1.93	0.65
1:A:298:MET:HB2	1:A:429:GLU:HG2	1.77	0.65
1:B:617:SER:HB3	2:B:2890:HOH:O	1.97	0.65
1:A:642:PRO:HG3	1:A:743:HIS:CE1	2.32	0.65
1:A:323:PRO:HA	1:A:362:SER:HB3	1.79	0.64
1:A:327:GLU:O	1:A:331:ARG:HG3	1.98	0.64
1:A:309:SER:OG	1:A:574:ILE:HG23	1.98	0.63
1:B:429:GLU:O	1:B:432:LYS:HG3	1.98	0.62
1:B:672:THR:HG22	1:B:688:PHE:HZ	1.63	0.62
1:A:420:GLY:H	1:B:349:ASN:ND2	1.98	0.62
1:A:642:PRO:HD3	1:A:746:ALA:CB	2.30	0.61
1:B:350:GLN:NE2	1:B:396:GLU:HG3	2.16	0.61
1:B:651:ILE:HG22	1:B:652:VAL:H	1.65	0.60
1:A:230:VAL:O	1:A:234:VAL:HG23	2.02	0.60
1:A:512:THR:O	1:A:513:SER:HB2	2.02	0.60
1:A:520:MET:CE	1:A:549:ARG:HB2	2.27	0.60
1:B:246:ALA:O	1:B:249:ALA:HB3	2.02	0.60
1:A:417:PRO:HG2	1:B:348:PRO:HB2	1.84	0.59
1:A:395:LEU:O	1:A:399:ARG:HG3	2.02	0.59
1:A:643:LYS:CB	1:A:651:ILE:HB	2.33	0.59
1:A:260:PRO:HG3	1:A:273:ASP:HB3	1.85	0.59
1:A:350:GLN:NE2	1:A:396:GLU:HG3	2.18	0.59
1:B:243:GLU:C	1:B:245:GLU:H	2.05	0.59
1:B:520:MET:CE	1:B:549:ARG:HB2	2.33	0.58
1:B:444:GLY:H	1:B:500:LYS:NZ	2.02	0.58
1:B:573:GLN:H	1:B:573:GLN:NE2	2.01	0.58
1:B:230:VAL:HG23	1:B:268:ARG:O	2.04	0.58
1:B:395:LEU:O	1:B:399:ARG:HG3	2.04	0.58
1:B:672:THR:HG22	1:B:688:PHE:CZ	2.39	0.58
1:A:237:LEU:HD13	1:A:250:LEU:HG	1.86	0.57
1:A:238:GLN:HB3	1:A:246:ALA:CB	2.34	0.57
1:B:350:GLN:HE22	1:B:396:GLU:HG3	1.69	0.57
1:B:727:LYS:HE3	1:B:731:ARG:NH2	2.20	0.57
1:A:630:ARG:NH1	1:A:630:ARG:HB2	2.19	0.57
1:B:537:ASN:HB3	1:B:615:PHE:O	2.05	0.57
1:A:672:THR:HG22	1:A:688:PHE:HZ	1.69	0.57
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.86	0.57
1:B:256:GLU:O	1:B:265:LYS:HE3	2.05	0.56
1:B:755:GLN:HG2	2:B:2656:HOH:O	2.06	0.56
1:A:605:PRO:HD2	1:A:608:LEU:HD12	1.85	0.56
1:A:701:ARG:HE	1:A:718:GLN:NE2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:GLU:O	1:B:331:ARG:HG3	2.06	0.55
1:B:652:VAL:O	1:B:654:PRO:HD3	2.05	0.55
1:A:642:PRO:HD3	1:A:746:ALA:HB2	1.87	0.55
1:B:394:SER:O	1:B:398:GLN:HG3	2.06	0.55
1:A:533:GLN:NE2	2:A:2320:HOH:O	2.40	0.55
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.89	0.55
1:B:605:PRO:HD2	1:B:608:LEU:HD12	1.88	0.55
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.72	0.54
1:A:350:GLN:HE22	1:A:396:GLU:HG3	1.72	0.54
1:A:672:THR:HG22	1:A:688:PHE:CZ	2.43	0.54
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.22	0.54
1:A:438:LYS:HE3	1:A:520:MET:HE1	1.89	0.54
1:B:241:GLN:HE22	1:B:730:TYR:N	2.04	0.54
1:A:710:SER:O	1:A:711:SER:HB2	2.08	0.54
1:B:234:VAL:O	1:B:238:GLN:HG2	2.08	0.54
1:A:391:ASN:HD21	1:A:393:CYS:HB2	1.72	0.54
1:A:211:ARG:HB3	1:A:213:GLU:OE2	2.07	0.53
1:B:261:SER:O	1:B:265:LYS:HB2	2.08	0.53
1:A:406:ARG:NH2	1:B:360:PHE:O	2.42	0.53
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.36	0.53
1:B:651:ILE:HG22	1:B:652:VAL:N	2.23	0.53
1:A:728:GLN:NE2	1:A:754:ILE:H	2.06	0.53
1:B:230:VAL:O	1:B:234:VAL:HG23	2.07	0.53
1:A:643:LYS:C	1:A:651:ILE:HG13	2.29	0.53
1:B:659:GLU:HG3	1:B:701:ARG:HB3	1.90	0.53
1:A:727:LYS:HE3	1:A:731:ARG:NH2	2.24	0.53
1:A:298:MET:CB	1:A:429:GLU:HG2	2.40	0.52
1:B:298:MET:CB	1:B:429:GLU:HG2	2.40	0.52
1:B:376:TYR:HA	1:B:379:LYS:HG2	1.90	0.52
1:B:710:SER:O	1:B:711:SER:HB2	2.09	0.52
1:A:642:PRO:HG2	1:A:716:ILE:CG2	2.40	0.52
1:B:675:ILE:HG12	1:B:684:TRP:NE1	2.24	0.52
1:B:630:ARG:NH1	1:B:630:ARG:HB2	2.25	0.52
1:A:228:LEU:HD13	1:A:233:LEU:HD13	1.92	0.52
1:A:659:GLU:HG3	1:A:701:ARG:HB3	1.90	0.52
1:A:376:TYR:HA	1:A:379:LYS:HG2	1.90	0.52
1:A:234:VAL:O	1:A:238:GLN:HG2	2.10	0.51
1:A:240:GLN:HE22	1:A:751:LYS:NZ	2.07	0.51
1:A:388:SER:HA	1:A:438:LYS:HB3	1.92	0.51
1:A:492:LEU:HA	1:A:495:MET:HE2	1.92	0.51
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ASP:O	1:A:613:THR:HG22	2.10	0.51
1:A:670:ARG:HG2	1:A:690:PHE:CE2	2.46	0.51
1:B:311:HIS:CD2	1:B:552:PRO:HD2	2.45	0.51
1:B:438:LYS:HE3	1:B:520:MET:CE	2.37	0.51
1:A:420:GLY:N	1:B:349:ASN:HD21	2.09	0.51
1:B:728:GLN:NE2	1:B:754:ILE:H	2.08	0.51
1:A:442:LEU:HB2	1:A:493:SER:OG	2.11	0.50
1:A:227:THR:HG22	1:A:270:MET:N	2.26	0.50
1:B:388:SER:HA	1:B:438:LYS:HB3	1.93	0.50
1:A:415:ASP:O	1:A:497:ILE:HD11	2.12	0.50
1:A:238:GLN:HB3	1:A:246:ALA:HB3	1.93	0.50
1:A:420:GLY:H	1:B:349:ASN:HD21	1.59	0.50
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.40	0.50
1:B:662:GLY:HA3	2:B:2796:HOH:O	2.11	0.49
1:B:243:GLU:C	1:B:245:GLU:N	2.65	0.49
1:B:492:LEU:HA	1:B:495:MET:HE2	1.94	0.49
1:B:652:VAL:HG12	1:B:654:PRO:HG3	1.94	0.49
1:B:246:ALA:H	1:B:250:LEU:HB2	1.77	0.49
1:A:240:GLN:HE22	1:A:751:LYS:HZ1	1.60	0.48
1:A:507:PHE:O	1:A:508:SER:HB3	2.13	0.48
1:B:672:THR:CG2	1:B:688:PHE:HZ	2.27	0.48
1:A:290:ALA:O	1:A:293:ARG:HG2	2.13	0.48
1:A:429:GLU:O	1:A:432:LYS:HG3	2.12	0.48
1:B:439:GLY:HA2	2:B:3008:HOH:O	2.13	0.48
1:B:610:ASP:O	1:B:613:THR:HG22	2.14	0.48
1:A:692:VAL:HG21	1:A:723:TRP:CZ3	2.48	0.48
1:B:516:ALA:HB1	1:B:518:TYR:CE1	2.49	0.48
1:B:373:ILE:O	1:B:377:ALA:HB2	2.14	0.47
1:A:228:LEU:O	1:A:269:GLN:HA	2.13	0.47
1:A:628:PRO:HA	1:A:692:VAL:O	2.15	0.47
1:A:639:GLN:HG2	1:A:747:THR:OG1	2.15	0.47
1:A:661:HIS:O	1:A:698:ALA:HA	2.14	0.47
1:B:350:GLN:HE22	1:B:396:GLU:CG	2.28	0.47
1:A:573:GLN:NE2	1:A:573:GLN:N	2.62	0.46
1:B:310:SER:HB2	1:B:337:CYS:SG	2.55	0.46
1:A:205:TYR:HB3	1:A:209:THR:OG1	2.15	0.46
1:A:350:GLN:HE22	1:A:396:GLU:CG	2.29	0.46
1:B:415:ASP:C	1:B:497:ILE:HD11	2.36	0.46
1:A:651:ILE:O	1:A:652:VAL:HG13	2.16	0.46
1:A:652:VAL:HG11	1:A:677:ASN:HD22	1.80	0.46
1:B:661:HIS:O	1:B:698:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HB	1:A:269:GLN:NE2	2.30	0.46
1:A:632:ARG:HH12	1:A:755:GLN:HG3	1.80	0.46
1:B:300:GLN:HB2	1:B:305:TYR:CE1	2.50	0.46
1:B:236:PHE:CD1	1:B:240:GLN:HG3	2.50	0.45
1:B:692:VAL:HG21	1:B:723:TRP:CZ3	2.51	0.45
1:A:254:LEU:HD22	1:A:278:TYR:CD1	2.52	0.45
1:A:373:ILE:O	1:A:377:ALA:HB2	2.17	0.45
1:B:642:PRO:HD3	1:B:746:ALA:HB2	1.99	0.45
1:B:712:LYS:HD3	1:B:713:ASN:N	2.32	0.45
1:A:712:LYS:HD3	1:A:713:ASN:N	2.32	0.45
1:B:290:ALA:O	1:B:293:ARG:HG2	2.17	0.45
1:B:670:ARG:HG2	1:B:690:PHE:CE2	2.51	0.45
1:A:672:THR:CG2	1:A:688:PHE:HZ	2.30	0.44
1:B:415:ASP:O	1:B:497:ILE:HD11	2.17	0.44
1:A:205:TYR:HA	1:A:208:LEU:HB3	1.99	0.44
1:B:660:ILE:CD1	1:B:700:VAL:HG22	2.48	0.44
1:B:378:PHE:HA	1:B:381:SER:O	2.18	0.44
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.82	0.44
1:A:263:THR:O	1:A:267:GLN:HG3	2.18	0.44
1:B:628:PRO:HA	1:B:692:VAL:O	2.18	0.44
1:A:642:PRO:HG2	1:A:716:ILE:HG23	1.99	0.43
1:B:384:PRO:HG3	1:B:431:LEU:HB2	2.00	0.43
1:A:537:ASN:HB3	1:A:615:PHE:O	2.18	0.43
1:A:259:GLU:OE2	1:A:261:SER:HB3	2.18	0.43
1:A:652:VAL:HG11	1:A:677:ASN:ND2	2.33	0.43
1:B:525:GLU:HG2	1:B:553:ALA:HB2	2.00	0.43
1:A:310:SER:HB2	1:A:337:CYS:SG	2.59	0.43
1:A:734:HIS:HE1	2:A:1821:HOH:O	2.01	0.43
1:A:438:LYS:HE3	1:A:520:MET:CE	2.47	0.43
1:B:355:TYR:CZ	1:B:357:GLY:HA2	2.54	0.42
1:B:594:GLN:HA	1:B:594:GLN:NE2	2.34	0.42
1:A:537:ASN:O	1:A:541:ARG:HG3	2.19	0.42
1:A:593:PHE:O	1:A:598:GLY:HA2	2.19	0.42
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.47	0.42
1:A:504:PHE:HB3	1:A:527:ARG:NH2	2.34	0.42
1:B:241:GLN:HA	1:B:241:GLN:NE2	2.35	0.42
1:A:655:LYS:HD2	1:A:674:VAL:HG22	2.00	0.42
1:A:706:ASP:HB3	1:A:714:ASP:HB2	2.00	0.42
1:A:238:GLN:O	1:A:242:ARG:HA	2.19	0.42
1:B:322:GLY:HA3	2:B:2504:HOH:O	2.19	0.42
1:A:728:GLN:HE21	1:A:754:ILE:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ILE:CD1	1:A:700:VAL:HG22	2.50	0.42
1:B:653:ASP:OD2	1:B:676:THR:HA	2.19	0.42
1:B:207:MET:HA	1:B:210:GLN:HE21	1.83	0.42
1:A:206:LYS:HA	1:A:210:GLN:HG3	2.01	0.41
1:A:233:LEU:HD23	1:A:251:ALA:HB1	2.02	0.41
1:A:653:ASP:OD2	1:A:676:THR:HA	2.19	0.41
1:B:248:PRO:O	1:B:252:LEU:HG	2.20	0.41
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.56	0.41
1:A:542:HIS:HE1	2:A:2411:HOH:O	2.02	0.41
1:B:641:LEU:HD12	1:B:641:LEU:HA	1.88	0.41
1:B:706:ASP:HB3	1:B:714:ASP:HB2	2.01	0.41
1:A:632:ARG:NH1	1:A:755:GLN:HG3	2.35	0.41
1:B:233:LEU:O	1:B:237:LEU:HG	2.20	0.41
1:A:300:GLN:HB2	1:A:305:TYR:CE1	2.55	0.41
1:B:403:ARG:HG3	1:B:403:ARG:HH11	1.86	0.41
1:A:394:SER:O	1:A:398:GLN:HG3	2.21	0.41
1:A:653:ASP:HA	1:A:675:ILE:O	2.21	0.41
1:B:209:THR:HG22	1:B:209:THR:O	2.21	0.41
1:B:241:GLN:HE21	1:B:241:GLN:N	2.19	0.41
1:B:728:GLN:HE21	1:B:754:ILE:H	1.68	0.41
1:A:291:HIS:HE1	1:A:724:ASN:O	2.04	0.40
1:A:378:PHE:HA	1:A:381:SER:O	2.22	0.40
1:B:593:PHE:O	1:B:598:GLY:HA2	2.21	0.40
1:B:390:GLU:HG2	1:B:392:HIS:NE2	2.35	0.40
1:A:642:PRO:HG2	1:A:716:ILE:HG22	2.03	0.40
1:A:259:GLU:HA	1:A:260:PRO:HD2	1.89	0.40
1:B:642:PRO:HG3	1:B:743:HIS:CE1	2.57	0.40
1:B:676:THR:HG22	1:B:677:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/622 (80%)	458 (92%)	31 (6%)	10 (2%)	7	9
1	B	496/622 (80%)	462 (93%)	29 (6%)	5 (1%)	15	23
All	All	995/1244 (80%)	920 (92%)	60 (6%)	15 (2%)	10	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	SER
1	A	711	SER
1	B	711	SER
1	A	508	SER
1	A	512	THR
1	A	652	VAL
1	B	443	GLY
1	B	508	SER
1	A	653	ASP
1	A	209	THR
1	B	444	GLY
1	A	509	SER
1	A	712	LYS
1	A	510	PRO
1	B	636	ILE

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	437/544 (80%)	418 (96%)	19 (4%)	29	46
1	B	435/544 (80%)	418 (96%)	17 (4%)	32	50
All	All	872/1088 (80%)	836 (96%)	36 (4%)	30	48

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	GLU

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Mol	Chain	Res	Type
1	A	216	ARG
1	A	227	THR
1	A	232	ARG
1	A	242	ARG
1	A	277	MET
1	A	388	SER
1	A	423	THR
1	A	434	LYS
1	A	436	LEU
1	A	539	PHE
1	A	573	GLN
1	A	622	GLN
1	A	639	GLN
1	A	641	LEU
1	A	652	VAL
1	A	691	GLU
1	A	714	ASP
1	A	718	GLN
1	B	216	ARG
1	B	242	ARG
1	B	254	LEU
1	B	267	GLN
1	B	388	SER
1	B	423	THR
1	B	434	LYS
1	B	436	LEU
1	B	539	PHE
1	B	573	GLN
1	B	622	GLN
1	B	639	GLN
1	B	641	LEU
1	B	643	LYS
1	B	691	GLU
1	B	714	ASP
1	B	718	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	240	GLN
1	A	267	GLN

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Mol	Chain	Res	Type
1	A	269	GLN
1	A	304	HIS
1	A	312	ASN
1	A	350	GLN
1	A	416	GLN
1	A	515	GLN
1	A	542	HIS
1	A	573	GLN
1	A	594	GLN
1	A	639	GLN
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	B	241	GLN
1	B	312	ASN
1	B	349	ASN
1	B	350	GLN
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	594	GLN
1	B	671	GLN
1	B	718	GLN
1	B	728	GLN
1	B	734	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section 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.