



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:16 pm BST

PDB ID : 1QAT
Title : 1-PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE PHOSPHODI-
ESTERASE DELTA COMPLEX WITH SAMARIUM (III) CHLORIDE
Authors : Grobler, J.A.; Hurley, J.H.
Deposited on : 1996-08-02
Resolution : 3.00 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
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

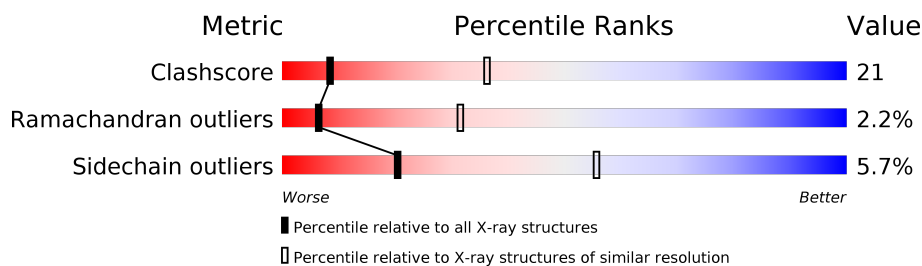
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	622	
1	B	622	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8022 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	509	Total	C	N	O	S	0	0	0
			4018	2536	704	756	22			
1	B	507	Total	C	N	O	S	0	0	0
			3999	2526	701	750	22			

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Sm	0	0
			3	3		
2	A	2	Total	Sm	0	0
			2	2		



4 Data and refinement statistics

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	61.60Å 75.10Å 86.40Å 66.40° 85.60° 89.80°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8022	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/4111	0.76	3/5568 (0.1%)
1	B	0.46	0/4090	0.76	4/5539 (0.1%)
All	All	0.46	0/8201	0.76	7/11107 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	A	331	ARG	NE-CZ-NH2	-13.87	113.36	120.30
1	B	331	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	B	331	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	A	331	ARG	CD-NE-CZ	7.13	133.59	123.60
1	B	331	ARG	CD-NE-CZ	6.89	133.24	123.60
1	B	207	MET	CG-SD-CE	6.14	110.03	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	TYR	Sidechain
1	B	305	TYR	Sidechain
1	B	383	TYR	Sidechain

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	4018	0	3941	166	0
1	B	3999	0	3916	166	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
All	All	8022	0	7857	330	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 21.

All (330) 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:206:LYS:HA	1:A:210:GLN:HG3	1.49	0.93
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.60	0.84
1:A:537:ASN:HD22	1:A:614:THR:HA	1.43	0.81
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.62	0.81
1:B:537:ASN:HD22	1:B:614:THR:HA	1.46	0.79
1:B:206:LYS:HA	1:B:209:THR:OG1	1.83	0.78
1:B:241:GLN:HE22	1:B:730:TYR:H	1.32	0.78
1:A:211:ARG:HB2	1:A:214:ILE:HB	1.65	0.76
1:B:309:SER:OG	1:B:574:ILE:HG23	1.86	0.76
1:A:350:GLN:HE22	1:A:396:GLU:HG3	1.52	0.75
1:B:350:GLN:HE22	1:B:396:GLU:HG3	1.52	0.74
1:B:648:LYS:HA	1:B:648:LYS:HE2	1.70	0.73
1:B:442:LEU:HG	1:B:488:LEU:HD23	1.69	0.72
1:B:245:GLU:HA	1:B:250:LEU:HD22	1.69	0.72
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.36	0.72
1:B:548:SER:H	1:B:573:GLN:HE21	1.38	0.71
1:B:289:LEU:HD12	1:B:292:ARG:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LYS:HD3	1:B:590:LEU:HD11	1.71	0.71
1:A:230:VAL:O	1:A:234:VAL:HG23	1.90	0.71
1:B:644:VAL:CG1	1:B:716:ILE:HG12	2.19	0.70
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.72	0.69
1:A:335:LYS:HD3	1:A:590:LEU:HD11	1.74	0.69
1:B:211:ARG:NH1	1:B:276:LEU:HD11	2.07	0.69
1:B:566:GLU:HG2	1:B:618:ARG:HH21	1.56	0.69
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.72	0.69
1:A:385:VAL:HG22	1:A:435:ILE:HG12	1.75	0.68
1:B:644:VAL:HG12	1:B:716:ILE:HG12	1.74	0.68
1:A:309:SER:OG	1:A:574:ILE:HG23	1.92	0.68
1:B:644:VAL:HG11	1:B:706:ASP:HB2	1.76	0.68
1:B:734:HIS:HA	1:B:747:THR:HG22	1.74	0.68
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.24	0.68
1:A:228:LEU:HB2	1:A:270:MET:HB3	1.76	0.68
1:B:610:ASP:HB3	1:B:613:THR:HB	1.76	0.68
1:A:536:GLY:HA3	1:A:616:ASN:HD22	1.59	0.67
1:B:399:ARG:O	1:B:403:ARG:HG2	1.95	0.67
1:B:385:VAL:HG22	1:B:435:ILE:HG12	1.77	0.67
1:A:610:ASP:HB3	1:A:613:THR:HB	1.77	0.67
1:B:605:PRO:HD2	1:B:608:LEU:HD12	1.76	0.67
1:A:701:ARG:HE	1:A:718:GLN:HE21	1.42	0.66
1:A:548:SER:H	1:A:573:GLN:HE21	1.43	0.66
1:A:566:GLU:HG2	1:A:618:ARG:HH21	1.61	0.65
1:B:652:VAL:O	1:B:677:ASN:HA	1.97	0.65
1:A:238:GLN:HB3	1:A:246:ALA:HB3	1.79	0.65
1:B:536:GLY:HA3	1:B:616:ASN:HD22	1.61	0.65
1:A:395:LEU:O	1:A:399:ARG:HG3	1.97	0.64
1:A:399:ARG:O	1:A:403:ARG:HG2	1.98	0.64
1:A:734:HIS:HA	1:A:747:THR:HG22	1.78	0.64
1:B:324:SER:H	1:B:362:SER:HB3	1.62	0.64
1:A:324:SER:H	1:A:362:SER:HB3	1.61	0.64
1:B:395:LEU:O	1:B:399:ARG:HG3	1.98	0.64
1:B:652:VAL:HG12	1:B:653:ASP:N	2.13	0.64
1:B:703:MET:HG2	1:B:718:GLN:HB3	1.79	0.64
1:A:605:PRO:HD2	1:A:608:LEU:HD12	1.80	0.64
1:B:228:LEU:HB2	1:B:270:MET:HB3	1.79	0.64
1:B:593:PHE:O	1:B:598:GLY:HA2	1.98	0.63
1:B:437:LEU:HD12	1:B:495:MET:HB3	1.80	0.63
1:A:651:ILE:HB	1:A:677:ASN:OD1	1.98	0.63
1:A:238:GLN:HB3	1:A:246:ALA:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:CD1	1:A:240:GLN:HG3	2.35	0.61
1:A:228:LEU:HD13	1:A:233:LEU:HD13	1.81	0.61
1:A:593:PHE:O	1:A:598:GLY:HA2	2.00	0.61
1:B:292:ARG:O	1:B:597:GLY:HA2	2.01	0.61
1:B:438:LYS:HE3	1:B:520:MET:HE2	1.81	0.61
1:A:437:LEU:HD12	1:A:495:MET:HB3	1.82	0.61
1:A:236:PHE:HD1	1:A:240:GLN:HG3	1.66	0.61
1:B:300:GLN:HB2	1:B:305:TYR:CE1	2.36	0.61
1:B:373:ILE:O	1:B:377:ALA:HB2	2.01	0.61
1:B:256:GLU:HA	1:B:265:LYS:HE3	1.82	0.60
1:B:301:PRO:HD2	1:B:304:HIS:ND1	2.17	0.60
1:A:373:ILE:O	1:A:377:ALA:HB2	2.01	0.59
1:A:256:GLU:HA	1:A:265:LYS:HE3	1.82	0.59
1:A:350:GLN:NE2	1:A:396:GLU:HG3	2.16	0.59
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.84	0.59
1:A:642:PRO:HD2	1:A:716:ILE:HG22	1.84	0.59
1:A:227:THR:HG22	1:A:269:GLN:HB3	1.84	0.59
1:A:642:PRO:HG2	1:A:743:HIS:CE1	2.37	0.59
1:B:350:GLN:NE2	1:B:396:GLU:HG3	2.17	0.59
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.00	0.59
1:B:536:GLY:HA3	1:B:616:ASN:ND2	2.17	0.58
1:A:300:GLN:HB2	1:A:305:TYR:CE2	2.38	0.58
1:A:692:VAL:HG21	1:A:723:TRP:CZ3	2.38	0.58
1:A:411:PRO:O	1:A:434:LYS:HE2	2.03	0.58
1:A:537:ASN:ND2	1:A:614:THR:HA	2.17	0.58
1:A:395:LEU:HD22	1:A:489:VAL:HG13	1.86	0.58
1:A:590:LEU:O	1:A:594:GLN:HG2	2.03	0.58
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.69	0.58
1:A:729:GLY:O	1:A:751:LYS:HA	2.03	0.58
1:B:729:GLY:O	1:B:751:LYS:HA	2.02	0.58
1:A:652:VAL:O	1:A:677:ASN:HA	2.04	0.58
1:A:630:ARG:NH1	1:A:630:ARG:HB2	2.20	0.57
1:B:590:LEU:O	1:B:594:GLN:HG2	2.03	0.57
1:A:596:ASN:ND2	1:A:599:CYS:SG	2.77	0.57
1:B:311:HIS:HB2	1:B:576:ALA:HB1	1.86	0.57
1:B:594:GLN:HE21	1:B:594:GLN:HA	1.69	0.57
1:B:218:PHE:CE1	1:B:228:LEU:HG	2.40	0.57
1:B:411:PRO:O	1:B:434:LYS:HE2	2.04	0.57
1:B:728:GLN:NE2	1:B:754:ILE:H	2.03	0.57
1:A:263:THR:O	1:A:267:GLN:HG3	2.05	0.57
1:B:610:ASP:O	1:B:613:THR:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD11	1:A:254:LEU:HD12	1.86	0.57
1:A:292:ARG:O	1:A:597:GLY:HA2	2.05	0.57
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.87	0.56
1:A:313:THR:HB	1:A:329:TYR:CE1	2.40	0.56
1:A:536:GLY:HA3	1:A:616:ASN:ND2	2.20	0.56
1:A:323:PRO:HA	1:A:362:SER:HB2	1.86	0.56
1:B:320:LEU:HD11	1:B:557:THR:HG21	1.88	0.56
1:B:548:SER:N	1:B:573:GLN:HE21	2.03	0.55
1:A:214:ILE:HG13	1:A:276:LEU:HD13	1.88	0.55
1:B:652:VAL:HG12	1:B:653:ASP:H	1.69	0.55
1:B:701:ARG:NE	1:B:718:GLN:HE21	2.03	0.55
1:A:429:GLU:O	1:A:432:LYS:HG3	2.05	0.55
1:B:429:GLU:O	1:B:432:LYS:HG3	2.05	0.55
1:B:633:VAL:HG11	1:B:702:PHE:HE2	1.73	0.54
1:A:400:VAL:HG12	1:A:404:HIS:CD2	2.42	0.54
1:A:301:PRO:HD2	1:A:304:HIS:ND1	2.23	0.54
1:B:537:ASN:ND2	1:B:614:THR:HA	2.20	0.54
1:B:323:PRO:HA	1:B:362:SER:HB2	1.89	0.54
1:B:537:ASN:O	1:B:541:ARG:HG3	2.09	0.53
1:B:728:GLN:HE21	1:B:754:ILE:H	1.56	0.53
1:B:727:LYS:HE3	1:B:731:ARG:NH2	2.23	0.53
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.89	0.53
1:B:246:ALA:H	1:B:250:LEU:HB2	1.73	0.53
1:A:549:ARG:NH1	1:A:549:ARG:HG2	2.23	0.53
1:B:354:ILE:HD12	1:B:369:VAL:HG21	1.89	0.53
1:B:492:LEU:HA	1:B:495:MET:HE3	1.89	0.53
1:A:701:ARG:HE	1:A:718:GLN:NE2	2.06	0.53
1:B:258:TYR:OH	1:B:283:ASP:HB2	2.08	0.53
1:A:610:ASP:O	1:A:613:THR:HG22	2.08	0.53
1:B:400:VAL:HG12	1:B:404:HIS:CD2	2.43	0.53
1:B:313:THR:HB	1:B:329:TYR:CE2	2.43	0.53
1:A:346:ASP:HA	1:A:397:GLN:OE1	2.09	0.53
1:A:420:GLY:H	1:B:349:ASN:ND2	2.07	0.53
1:A:537:ASN:O	1:A:541:ARG:HG3	2.09	0.53
1:B:230:VAL:O	1:B:234:VAL:HG23	2.09	0.53
1:B:630:ARG:HB2	1:B:630:ARG:NH1	2.25	0.52
1:B:596:ASN:ND2	1:B:599:CYS:SG	2.82	0.52
1:A:728:GLN:NE2	1:A:754:ILE:H	2.08	0.52
1:A:297:ASP:OD1	1:A:300:GLN:HG2	2.09	0.52
1:B:644:VAL:C	1:B:646:LYS:H	2.13	0.52
1:A:282:ALA:HB1	1:A:289:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:LEU:N	1:B:436:LEU:HD23	2.24	0.52
1:A:648:LYS:HE2	1:A:648:LYS:HA	1.90	0.52
1:A:237:LEU:HD23	1:A:241:GLN:HG3	1.92	0.52
1:B:692:VAL:HG21	1:B:723:TRP:CZ3	2.45	0.51
1:B:330:ILE:HG12	1:B:376:TYR:CD2	2.45	0.51
1:A:549:ARG:HG2	1:A:549:ARG:HH11	1.76	0.51
1:B:304:HIS:O	1:B:603:LEU:HD12	2.10	0.51
1:B:346:ASP:HA	1:B:397:GLN:OE1	2.11	0.51
1:B:736:LEU:HA	1:B:742:GLN:HA	1.91	0.51
1:A:206:LYS:HA	1:A:210:GLN:CG	2.30	0.51
1:A:311:HIS:HB2	1:A:576:ALA:HB1	1.93	0.51
1:A:703:MET:HG2	1:A:718:GLN:HB3	1.91	0.51
1:A:736:LEU:HA	1:A:742:GLN:HA	1.91	0.51
1:A:548:SER:N	1:A:573:GLN:HE21	2.07	0.51
1:B:644:VAL:HG21	1:B:706:ASP:OD2	2.10	0.51
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.36	0.51
1:A:211:ARG:HB3	1:A:213:GLU:OE2	2.10	0.51
1:A:638:GLY:HA2	1:A:748:LEU:HA	1.93	0.51
1:B:211:ARG:HB2	1:B:213:GLU:OE2	2.10	0.51
1:B:355:TYR:CZ	1:B:357:GLY:HA2	2.46	0.51
1:B:257:ARG:HD2	1:B:258:TYR:CZ	2.45	0.51
1:A:354:ILE:HD12	1:A:369:VAL:HG21	1.93	0.50
1:A:492:LEU:HA	1:A:495:MET:HE3	1.92	0.50
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.26	0.50
1:A:523:PHE:HD1	1:A:527:ARG:HD3	1.76	0.50
1:B:650:SER:O	1:B:651:ILE:HG13	2.11	0.50
1:B:395:LEU:HD22	1:B:489:VAL:HG13	1.94	0.50
1:A:300:GLN:HG3	1:A:603:LEU:HD11	1.94	0.50
1:A:727:LYS:HE3	1:A:731:ARG:NH2	2.27	0.50
1:A:396:GLU:O	1:A:400:VAL:HG23	2.11	0.49
1:B:297:ASP:OD1	1:B:300:GLN:HG2	2.12	0.49
1:B:444:GLY:HA2	1:B:500:LYS:HZ1	1.76	0.49
1:A:421:VAL:HG11	1:A:426:PRO:HD3	1.94	0.49
1:B:429:GLU:HA	1:B:432:LYS:HG3	1.93	0.49
1:A:355:TYR:CZ	1:A:357:GLY:HA2	2.48	0.49
1:A:429:GLU:HA	1:A:432:LYS:HG3	1.92	0.49
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.38	0.49
1:A:313:THR:O	1:A:328:ALA:HB1	2.12	0.49
1:A:436:LEU:N	1:A:436:LEU:HD23	2.28	0.49
1:B:438:LYS:CE	1:B:520:MET:HE2	2.42	0.49
1:B:396:GLU:O	1:B:400:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ARG:HH11	1:A:618:ARG:HG3	1.76	0.49
1:A:290:ALA:O	1:A:293:ARG:HG2	2.13	0.48
1:B:427:SER:OG	1:B:430:GLN:HG3	2.13	0.48
1:A:258:TYR:CE1	1:A:281:SER:HB2	2.48	0.48
1:A:630:ARG:HH11	1:A:630:ARG:HB2	1.78	0.48
1:A:633:VAL:HG11	1:A:702:PHE:HE2	1.78	0.48
1:B:234:VAL:O	1:B:238:GLN:HG2	2.13	0.48
1:B:549:ARG:HG2	1:B:549:ARG:NH1	2.28	0.48
1:B:523:PHE:HD1	1:B:527:ARG:HD3	1.78	0.48
1:B:548:SER:H	1:B:573:GLN:NE2	2.10	0.48
1:A:701:ARG:NE	1:A:718:GLN:HE21	2.10	0.48
1:B:555:TRP:HE3	1:B:555:TRP:O	1.96	0.48
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.44	0.48
1:B:245:GLU:HA	1:B:250:LEU:CD2	2.43	0.48
1:B:438:LYS:CD	1:B:520:MET:HE2	2.44	0.48
1:B:675:ILE:HG12	1:B:684:TRP:NE1	2.29	0.48
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.48	0.47
1:B:292:ARG:C	1:B:597:GLY:HA2	2.35	0.47
1:B:256:GLU:O	1:B:265:LYS:HE3	2.13	0.47
1:A:728:GLN:HE21	1:A:754:ILE:H	1.62	0.47
1:B:528:ALA:O	1:B:532:LEU:HG	2.14	0.47
1:B:643:LYS:O	1:B:645:ASN:N	2.47	0.47
1:A:438:LYS:CD	1:A:520:MET:HE2	2.45	0.47
1:A:628:PRO:HB3	1:A:693:THR:HA	1.97	0.47
1:B:652:VAL:CG1	1:B:653:ASP:N	2.78	0.47
1:A:259:GLU:OE2	1:A:261:SER:HB3	2.15	0.47
1:A:438:LYS:HE3	1:A:520:MET:HE2	1.97	0.46
1:B:594:GLN:HE21	1:B:594:GLN:CA	2.28	0.46
1:B:643:LYS:H	1:B:643:LYS:HD2	1.81	0.46
1:A:562:TYR:CE1	1:A:577:LEU:HD23	2.51	0.46
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.28	0.46
1:B:241:GLN:N	1:B:241:GLN:HE21	2.14	0.46
1:B:300:GLN:HB2	1:B:305:TYR:CZ	2.51	0.46
1:A:388:SER:HA	1:A:438:LYS:HB3	1.98	0.46
1:B:258:TYR:O	1:B:260:PRO:HD3	2.15	0.46
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.81	0.46
1:B:618:ARG:HG3	1:B:618:ARG:HH11	1.78	0.46
1:A:555:TRP:O	1:A:555:TRP:HE3	1.98	0.46
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.51	0.45
1:A:330:ILE:HG12	1:A:376:TYR:CD2	2.51	0.45
1:B:228:LEU:HD12	1:B:270:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:THR:O	1:B:328:ALA:HB1	2.15	0.45
1:B:369:VAL:O	1:B:373:ILE:HG13	2.16	0.45
1:A:427:SER:OG	1:A:430:GLN:HG3	2.16	0.45
1:B:525:GLU:OE2	1:B:556:ARG:NE	2.49	0.45
1:B:289:LEU:HA	1:B:292:ARG:HG2	1.98	0.45
1:A:441:LYS:HD2	1:A:496:ILE:O	2.17	0.45
1:B:415:ASP:C	1:B:497:ILE:HD11	2.37	0.45
1:B:630:ARG:HB2	1:B:630:ARG:HH11	1.82	0.45
1:B:638:GLY:HA2	1:B:748:LEU:HA	1.99	0.45
1:A:508:SER:O	1:A:509:SER:HB2	2.16	0.45
1:B:707:TYR:CE2	1:B:709:SER:HA	2.51	0.45
1:B:642:PRO:HD3	1:B:746:ALA:HB2	1.97	0.45
1:B:606:ALA:HA	1:B:609:ARG:HE	1.82	0.45
1:B:290:ALA:O	1:B:293:ARG:HG2	2.17	0.45
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.99	0.45
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.99	0.44
1:B:214:ILE:HG13	1:B:276:LEU:HD13	1.99	0.44
1:B:317:GLU:HB2	1:B:323:PRO:HD2	1.98	0.44
1:B:403:ARG:HG3	1:B:403:ARG:HH11	1.82	0.44
1:A:256:GLU:HA	1:A:265:LYS:CE	2.47	0.44
1:A:525:GLU:OE2	1:A:556:ARG:NE	2.49	0.44
1:A:235:THR:O	1:A:239:HIS:HB3	2.18	0.44
1:A:277:MET:O	1:A:281:SER:HB3	2.17	0.44
1:A:712:LYS:HG2	1:A:713:ASN:H	1.81	0.44
1:A:706:ASP:O	1:A:713:ASN:HA	2.17	0.44
1:B:388:SER:HA	1:B:438:LYS:HB3	2.00	0.44
1:B:652:VAL:CG1	1:B:653:ASP:H	2.28	0.44
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.53	0.44
1:B:324:SER:N	1:B:362:SER:HB3	2.32	0.44
1:B:364:ILE:HD12	1:B:369:VAL:HG22	1.99	0.44
1:B:228:LEU:HD13	1:B:233:LEU:HD13	2.00	0.44
1:B:489:VAL:HG23	1:B:492:LEU:H	1.81	0.44
1:B:739:ASN:ND2	1:B:741:ASP:CG	2.72	0.44
1:B:248:PRO:O	1:B:252:LEU:HD12	2.16	0.44
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.88	0.43
1:A:221:ALA:HB1	1:A:228:LEU:HD21	2.01	0.43
1:B:227:THR:HG22	1:B:271:THR:HG22	1.99	0.43
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.71	0.43
1:A:300:GLN:HB2	1:A:305:TYR:CZ	2.54	0.43
1:B:347:GLY:HA3	1:B:351:GLU:O	2.18	0.43
1:B:487:LYS:HG2	1:B:487:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:O	1:A:359:THR:HB	2.17	0.43
1:A:237:LEU:O	1:A:241:GLN:HB2	2.19	0.43
1:A:257:ARG:HG2	1:A:257:ARG:O	2.18	0.43
1:B:323:PRO:HA	1:B:362:SER:CB	2.48	0.43
1:A:317:GLU:HB2	1:A:323:PRO:HD2	2.00	0.43
1:A:308:SER:OG	1:A:337:CYS:HA	2.19	0.43
1:A:644:VAL:HG22	1:A:644:VAL:O	2.18	0.43
1:A:654:PRO:HD2	1:A:675:ILE:O	2.17	0.43
1:B:237:LEU:HD13	1:B:250:LEU:HD23	2.01	0.43
1:B:343:ASP:HA	1:B:390:GLU:HB3	2.01	0.43
1:A:343:ASP:HA	1:A:390:GLU:HB3	2.01	0.43
1:A:492:LEU:HD23	1:A:495:MET:CE	2.48	0.43
1:A:700:VAL:HG21	1:A:726:LEU:HD22	2.00	0.43
1:B:700:VAL:HG21	1:B:726:LEU:HD22	2.00	0.43
1:A:490:PRO:HD2	1:B:327:GLU:OE2	2.19	0.43
1:B:549:ARG:HG2	1:B:549:ARG:HH11	1.84	0.43
1:A:258:TYR:CE1	1:A:281:SER:CB	3.02	0.42
1:A:507:PHE:O	1:A:508:SER:HB3	2.18	0.42
1:B:246:ALA:CB	1:B:249:ALA:HB3	2.49	0.42
1:A:229:SER:OG	1:A:232:ARG:HB2	2.20	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.66	0.42
1:B:341:GLU:C	1:B:342:LEU:HD12	2.40	0.42
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.54	0.42
1:B:592:CYS:HB2	1:B:699:LEU:HD21	2.00	0.42
1:B:674:VAL:HG21	1:B:707:TYR:CG	2.54	0.42
1:A:618:ARG:HG3	1:A:618:ARG:NH1	2.34	0.42
1:B:296:GLN:HG3	1:B:596:ASN:OD1	2.20	0.42
1:B:507:PHE:O	1:B:508:SER:HB2	2.20	0.42
1:B:562:TYR:CE1	1:B:577:LEU:HD23	2.55	0.42
1:B:701:ARG:HH21	1:B:718:GLN:HG2	1.84	0.42
1:A:245:GLU:HB2	1:A:250:LEU:HD22	2.02	0.42
1:A:292:ARG:C	1:A:597:GLY:HA2	2.39	0.42
1:A:324:SER:HB2	1:A:362:SER:O	2.20	0.42
1:A:341:GLU:C	1:A:342:LEU:HD12	2.41	0.42
1:A:340:LEU:HB2	1:A:387:LEU:CD2	2.50	0.41
1:A:739:ASN:ND2	1:A:741:ASP:CG	2.74	0.41
1:B:537:ASN:HB3	1:B:615:PHE:O	2.20	0.41
1:A:260:PRO:HG3	1:A:273:ASP:CB	2.50	0.41
1:A:528:ALA:O	1:A:532:LEU:HG	2.19	0.41
1:B:442:LEU:HD21	1:B:488:LEU:HB3	2.02	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:SER:HA	1:A:549:ARG:O	2.20	0.41
1:B:421:VAL:HG11	1:B:426:PRO:HD3	2.02	0.41
1:B:310:SER:HB2	1:B:337:CYS:SG	2.60	0.41
1:A:606:ALA:HA	1:A:609:ARG:HE	1.86	0.41
1:A:255:ILE:O	1:A:259:GLU:HB3	2.21	0.41
1:A:304:HIS:O	1:A:603:LEU:HD12	2.21	0.41
1:B:618:ARG:HG3	1:B:618:ARG:NH1	2.35	0.41
1:B:645:ASN:O	1:B:647:ASN:N	2.53	0.41
1:A:288:SER:HA	1:A:727:LYS:HD2	2.02	0.41
1:A:652:VAL:HG12	1:A:653:ASP:N	2.35	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.86	0.41
1:A:415:ASP:C	1:A:497:ILE:HD11	2.40	0.41
1:B:218:PHE:HE1	1:B:228:LEU:HG	1.84	0.41
1:A:655:LYS:HB3	1:A:674:VAL:HG22	2.02	0.41
1:B:492:LEU:HD23	1:B:495:MET:CE	2.50	0.41
1:A:310:SER:HB2	1:A:337:CYS:SG	2.61	0.40
1:A:322:GLY:O	1:A:361:THR:HA	2.20	0.40
1:A:410:GLY:HA3	1:A:411:PRO:HD2	1.87	0.40
1:A:537:ASN:HB3	1:A:615:PHE:O	2.21	0.40
1:B:555:TRP:CE3	1:B:555:TRP:O	2.74	0.40
1:A:626:TRP:HH2	1:A:665:ARG:CZ	2.34	0.40
1:B:654:PRO:HD2	1:B:675:ILE:O	2.21	0.40
1:A:323:PRO:HA	1:A:362:SER:CB	2.50	0.40
1:A:654:PRO:HG2	1:A:678:ASN:O	2.20	0.40
1:B:255:ILE:HD13	1:B:255:ILE:HG21	1.85	0.40
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.57	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	505/622 (81%)	457 (90%)	37 (7%)	11 (2%)	6	31
1	B	501/622 (80%)	452 (90%)	38 (8%)	11 (2%)	6	31
All	All	1006/1244 (81%)	909 (90%)	75 (8%)	22 (2%)	6	31

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	THR
1	A	513	SER
1	A	647	ASN
1	B	444	GLY
1	B	644	VAL
1	B	646	LYS
1	A	508	SER
1	A	246	ALA
1	A	650	SER
1	A	677	ASN
1	A	678	ASN
1	B	677	ASN
1	B	678	ASN
1	B	709	SER
1	B	710	SER
1	A	442	LEU
1	A	288	SER
1	A	712	LYS
1	B	281	SER
1	B	288	SER
1	B	650	SER
1	B	443	GLY

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	441/544 (81%)	416 (94%)	25 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	437/544 (80%)	412 (94%)	25 (6%)	20	56
All	All	878/1088 (81%)	828 (94%)	50 (6%)	20	56

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	A	216	ARG
1	A	232	ARG
1	A	288	SER
1	A	313	THR
1	A	342	LEU
1	A	385	VAL
1	A	391	ASN
1	A	434	LYS
1	A	436	LEU
1	A	490	PRO
1	A	503	HIS
1	A	524	SER
1	A	539	PHE
1	A	573	GLN
1	A	592	CYS
1	A	594	GLN
1	A	622	GLN
1	A	639	GLN
1	A	641	LEU
1	A	691	GLU
1	A	708	ASP
1	A	713	ASN
1	A	714	ASP
1	A	718	GLN
1	B	211	ARG
1	B	215	ASP
1	B	216	ARG
1	B	252	LEU
1	B	254	LEU
1	B	277	MET
1	B	283	ASP
1	B	342	LEU
1	B	385	VAL
1	B	391	ASN
1	B	434	LYS

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Mol	Chain	Res	Type
1	B	436	LEU
1	B	490	PRO
1	B	503	HIS
1	B	524	SER
1	B	539	PHE
1	B	592	CYS
1	B	594	GLN
1	B	622	GLN
1	B	639	GLN
1	B	641	LEU
1	B	643	LYS
1	B	691	GLU
1	B	708	ASP
1	B	718	GLN

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

Mol	Chain	Res	Type
1	A	350	GLN
1	A	391	ASN
1	A	503	HIS
1	A	515	GLN
1	A	537	ASN
1	A	573	GLN
1	A	594	GLN
1	A	596	ASN
1	A	718	GLN
1	A	724	ASN
1	A	728	GLN
1	A	743	HIS
1	B	210	GLN
1	B	241	GLN
1	B	349	ASN
1	B	350	GLN
1	B	391	ASN
1	B	503	HIS
1	B	515	GLN
1	B	537	ASN
1	B	573	GLN
1	B	594	GLN
1	B	596	ASN
1	B	718	GLN

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Mol	Chain	Res	Type
1	B	728	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.