



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 06:44 am GMT

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)

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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

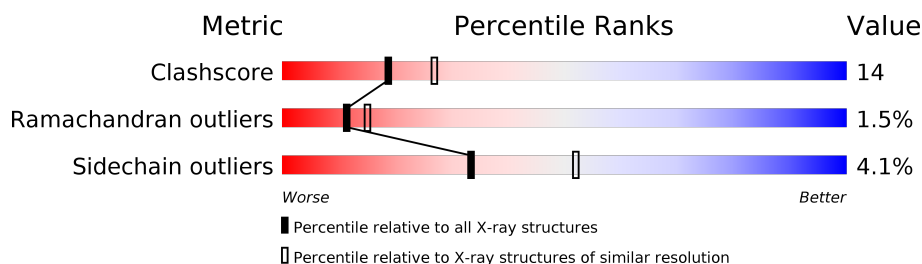
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122078	3953 (2.40-2.40)
Ramachandran outliers	120005	3894 (2.40-2.40)
Sidechain outliers	119972	3895 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 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.

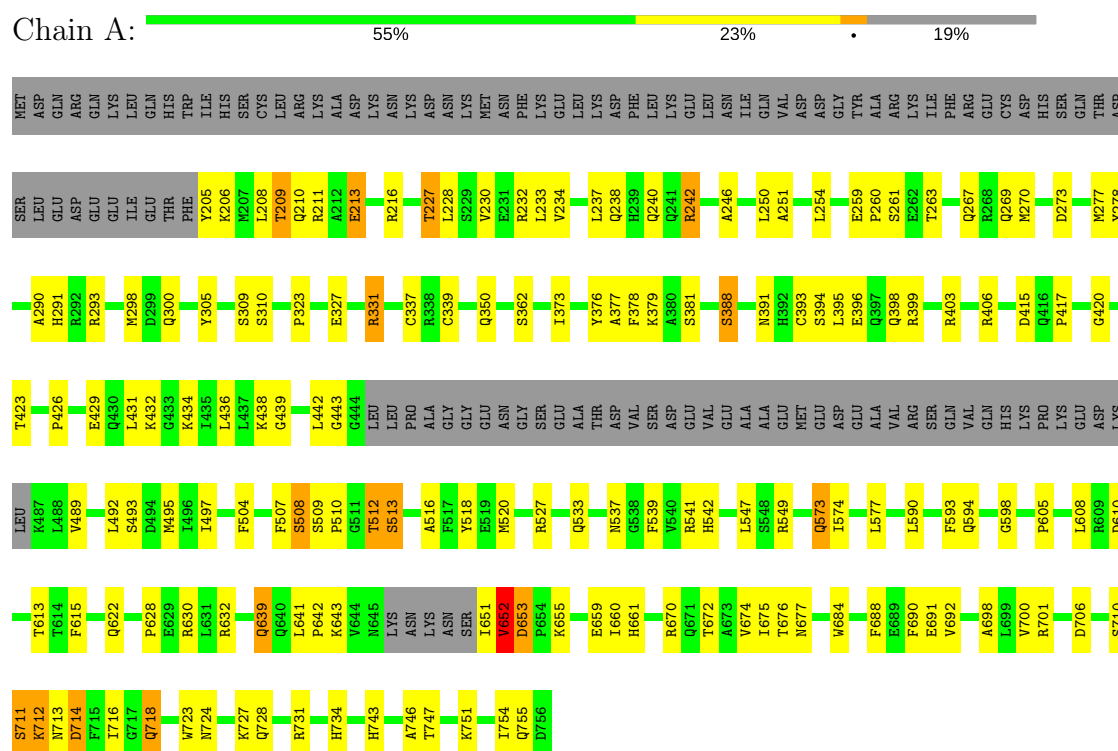
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	134	Total	O	0	0
			134	134		

3 Residue-property plots

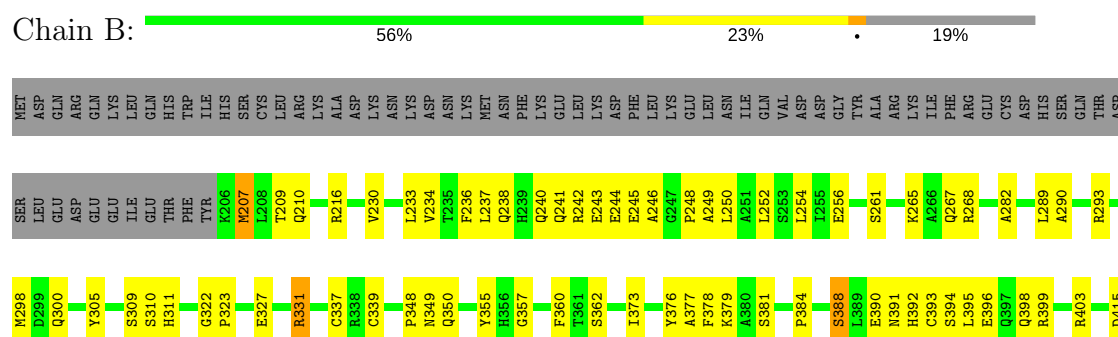
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



DY14	T423	L492	S616	P426	L496	P628	S617	I497	Q622	P629	S618	M495	K500	F504	F507	S608	S609	P510	GLY	THR	SER	Q443	Q444	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	ASP	K485
Q718	L493	M496	S619	I498	P623	S620	Q623	I499	Q624	P630	S621	M497	K501	F505	F508	S609	S610	P511	GLY	THR	SER	Q443	Q444	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	ASP	K485
W723	L494	M498	S622	I500	P624	S623	Q625	I501	Q626	P631	S624	M499	K502	F506	F509	S610	S611	P512	GLY	THR	SER	Q443	Q444	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	ASP	K485
K727	L495	M500	S625	I502	P625	S626	Q627	I503	Q628	P632	S627	M501	K503	F507	F510	S611	S612	P513	GLY	THR	SER	Q443	Q444	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	ASP	K485
Q728	L496	M502	S628	I504	P626	S629	Q629	I505	Q630	P633	S630	M503	K504	F508	F511	S612	S613	P514	GLY	THR	SER	Q443	Q444	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	ASP	K485
Y730	L497	M504	S630	I506	P627	S631	Q631	I507	Q632	P634	S632	M505	K505	F509	F512	S613	S614	P515	GLY	THR	SER	Q443	Q444	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	ASP	K485
R731	L498	M506	S632	I508	P628	S633	Q633	I509	Q634	P635	S634	M507	K506	F510	F513	S614	S615	P516	GLY	THR	SER	Q443	Q444	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	ASP	K485
H734	L499	M508	S634	I510	P629	S635	Q635	I511	Q636	P636	S635	M509	K507	F511	F514	S615	S616	P517	GLY	THR	SER	Q443	Q444	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	ASP	K485
H743	L500	M510	S636	I512	P630	S637	Q637	I513	Q638	P637	S636	M511	K508	F512	F515	S616	S617	P518	GLY	THR	SER	Q443	Q444	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	ASP	K485
A746	L501	M512	S638	I514	P631	S639	Q639	I515	Q640	P638	S637	M513	K509	F513	F516	S617	S618	P519	GLY	THR	SER	Q443	Q444	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	ASP	K485
I754	L502	M514	S640	I516	P632	S641	Q641	I517	Q642	P639	S638	M515	K510	F514	F517	S618	S619	P520	GLY	THR	SER	Q443	Q444	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	ASP	K485
Q755	L503	M516	S642	I518	P633	S643	Q643	I519	Q644	P640	S639	M517	K511	F515	F518	S619	S620	P521	GLY	THR	SER	Q443	Q444	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	ASP	K485
D756	L504	M518	S644	I520	P634	S645	Q645	I521	Q646	P641	S640	M519	K512	F516	F519	S620	S621	P522	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L505	M520	S646	I522	P635	S647	Q647	I523	Q648	P642	S641	M521	K513	F517	F520	S621	S622	P523	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L506	M522	S648	I524	P636	S649	Q649	I525	Q650	P643	S642	M523	K514	F518	F521	S622	S623	P524	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L507	M524	S650	I526	P637	S651	Q651	I527	Q652	P644	S643	M525	K515	F519	F522	S623	S624	P525	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L508	M526	S652	I528	P638	S653	Q653	I529	Q654	P645	S644	M527	K516	F520	F523	S624	S625	P526	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L509	M528	S654	I530	P639	S655	Q655	I531	Q656	P646	S645	M529	K517	F521	F524	S625	S626	P527	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L510	M530	S656	I532	P640	S657	Q657	I533	Q658	P647	S646	M531	K518	F522	F525	S626	S627	P528	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L511	M532	S658	I534	P641	S659	Q659	I535	Q660	P648	S647	M533	K519	F523	F526	S627	S628	P529	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L512	M534	S660	I536	P642	S661	Q661	I537	Q662	P649	S648	M535	K520	F524	F527	S628	S629	P530	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L513	M536	S662	I538	P643	S663	Q663	I539	Q664	P650	S649	M537	K521	F525	F528	S629	S630	P531	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L514	M538	S664	I540	P644	S665	Q665	I541	Q666	P651	S650	M539	K522	F526	F529	S630	S631	P532	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L515	M540	S666	I542	P645	S667	Q667	I543	Q668	P652	S651	M541	K523	F527	F530	S631	S632	P533	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L516	M542	S668	I544	P646	S669	Q669	I545	Q670	P653	S652	M543	K524	F528	F531	S632	S633	P534	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L517	M544	S670	I546	P647	S671	Q671	I547	Q672	P654	S653	M545	K525	F529	F532	S633	S634	P535	GLY	THR	SER	Q443	Q444	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	ASP	K485
	L518	M546	S672	I548	P648	S673	Q673	I549	Q674	P655	S654	M547	K526	F530	F533	S634	S635	P536	GLY	THR	SER	Q443	Q444	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														

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	61.10Å 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(°)	Ideal(°)
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:238:GLN:HB3	1:A:246:ALA:CB	2.34	0.57
1:A:237:LEU:HD13	1:A:250:LEU:HG	1.86	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:376:TYR:HA	1:B:379:LYS:HG2	1.90	0.52
1:B:298:MET:CB	1:B:429:GLU:HG2	2.40	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:HB2	1:B:630:ARG:NH1	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:507:PHE:O	1:A:508:SER:HB3	2.13	0.48
1:A:240:GLN:HE22	1:A:751:LYS:HZ1	1.60	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:712:LYS:HD3	1:B:713:ASN:N	2.32	0.45
1:B:642:PRO:HD3	1:B:746:ALA:HB2	1.99	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:NE2	1:B:594:GLN:HA	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:B:241:GLN:N	1:B:241:GLN:HE21	2.19	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:O	1:B:209:THR:HG22	2.21	0.41
1:B:728:GLN:HE21	1:B:754:ILE:H	1.68	0.41
1:A:378:PHE:HA	1:A:381:SER:O	2.22	0.40
1:A:291:HIS:HE1	1:A:724:ASN:O	2.04	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:676:THR:HG22	1:B:677:ASN:OD1	2.22	0.40
1:B:642:PRO:HG3	1:B:743:HIS:CE1	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	499/622 (80%)	458 (92%)	31 (6%)	10 (2%)	8	9
1	B	496/622 (80%)	462 (93%)	29 (6%)	5 (1%)	17	25
All	All	995/1244 (80%)	920 (92%)	60 (6%)	15 (2%)	11	15

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%)	32	49
1	B	435/544 (80%)	418 (96%)	17 (4%)	35	54
All	All	872/1088 (80%)	836 (96%)	36 (4%)	33	52

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

Some 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 carbohydrates 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.