Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 06:12 PM EST

PDB ID	:	3QR1
Title	:	Crystal Structure of L. pealei PLC21
Authors	:	Lyon, A.M.; Suddala, K.C.; Northup, J.K.; Tesmer, J.J.G.
Deposited on	:	2011-02-16
Resolution	:	3.20 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:

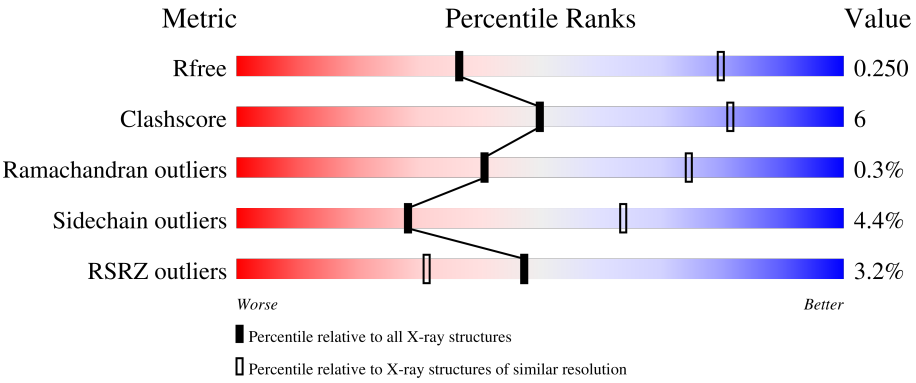
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	813	2% 81% 14%
1	D	813	4% 81% 13% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12526 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-BETA (PLC-BETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6262	4010	1044	1175	33			
1	D	775	Total	C	N	O	S	0	0	0
			6224	3986	1038	1167	33			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

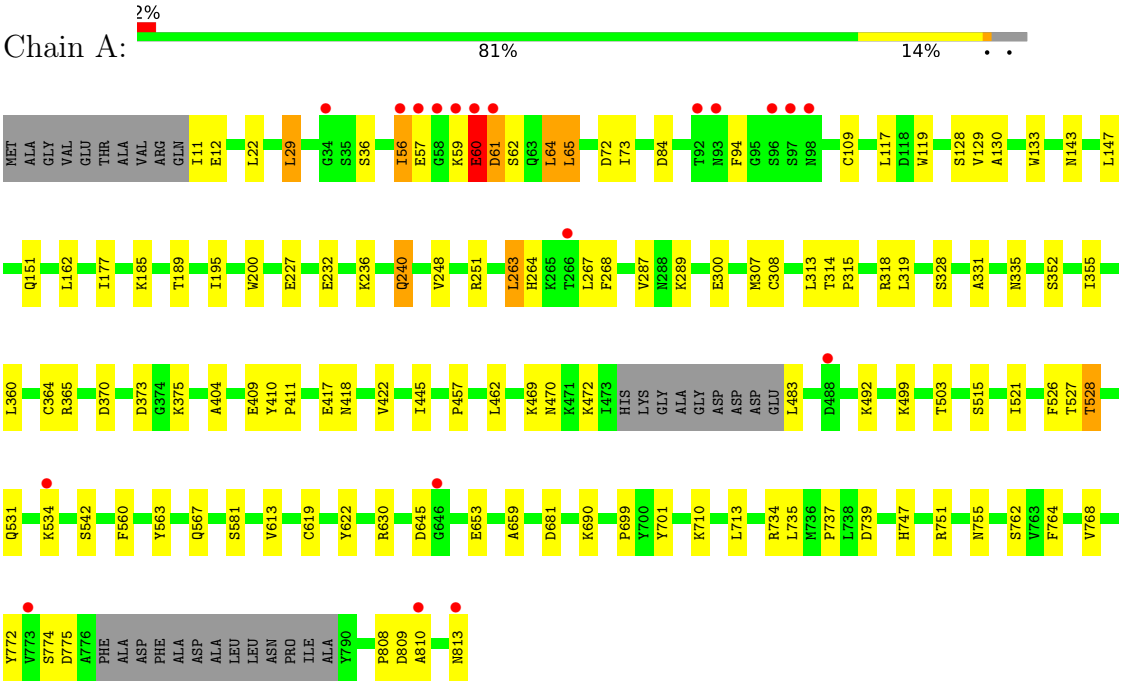
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	D	20	Total	O	0	0
			20	20		

3 Residue-property plots (i)

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 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.

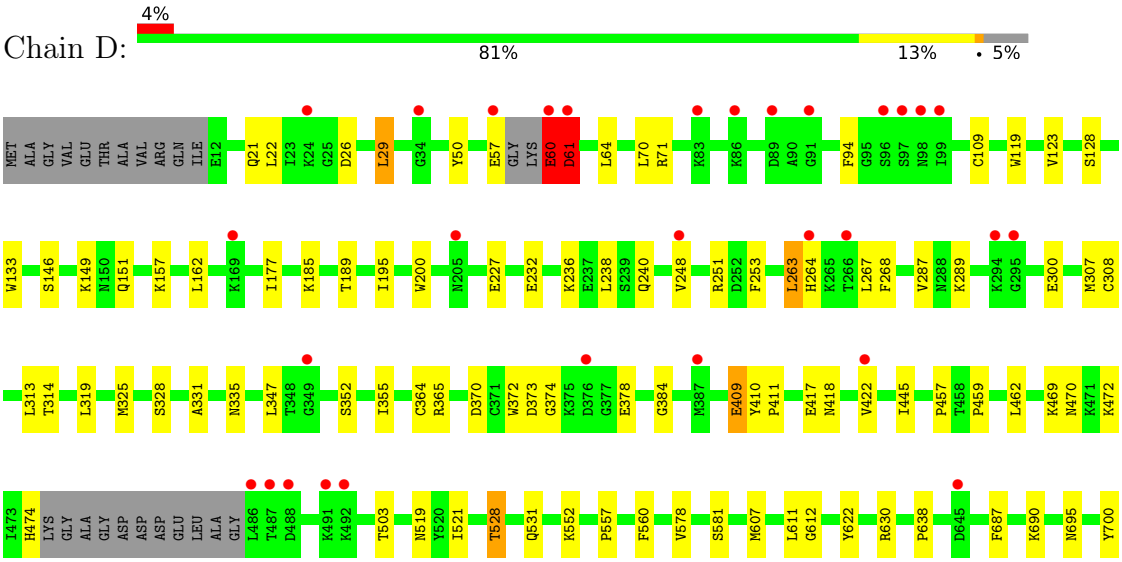
• Molecule 1: PHOSPHOLIPASE C-BETA (PLC-BETA)

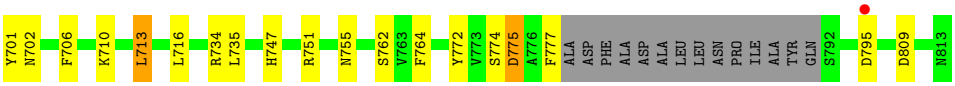
Chain A:



• Molecule 1: PHOSPHOLIPASE C-BETA (PLC-BETA)

Chain D:




Y701
N702
F706
K710
L713
L716
R734
L735
H747
R751
N755
S762
V763
F764
Y772
V773
S774
D775
A776
F777
ALA
ASP
PHE
ALA
ASP
ALA
LEU
LEU
ASN
PRO
ILE
ALA
TYR
GLN
S792
D795
D809
N813

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.37Å 148.87Å 151.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.20 29.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.97-3.20) 100.0 (29.97-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 3.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.258 0.211 , 0.250	Depositor DCC
R_{free} test set	1615 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12526	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.64	2/6400 (0.0%)	0.67	2/8643 (0.0%)
1	D	0.55	2/6362 (0.0%)	0.63	1/8591 (0.0%)
All	All	0.60	4/12762 (0.0%)	0.65	3/17234 (0.0%)

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	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	619	CYS	CB-SG	-5.99	1.72	1.81
1	A	60	GLU	CB-CG	5.61	1.62	1.52
1	D	409	GLU	CG-CD	5.58	1.60	1.51
1	D	60	GLU	CD-OE2	5.43	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	LEU	CA-CB-CG	5.86	128.78	115.30
1	D	61	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	65	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	GLU	Peptide
1	D	61	ASP	Peptide

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	6262	0	6240	77	0
1	D	6224	0	6192	72	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	18	0	0	2	0
3	D	20	0	0	1	0
All	All	12526	0	12432	144	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 6.

All (144) 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:747:HIS:HD2	1:A:764:PHE:HD1	1.09	0.98
1:A:747:HIS:CD2	1:A:764:PHE:HD1	1.87	0.90
1:D:747:HIS:HD2	1:D:764:PHE:HD1	1.15	0.90
1:D:747:HIS:CD2	1:D:764:PHE:HD1	1.90	0.90
1:D:528:THR:HG23	1:D:531:GLN:HB2	1.58	0.86
1:A:747:HIS:CD2	1:A:764:PHE:CD1	2.65	0.84
1:A:747:HIS:HD2	1:A:764:PHE:CD1	1.98	0.79
1:D:747:HIS:CD2	1:D:764:PHE:CD1	2.69	0.79
1:A:528:THR:HG23	1:A:531:GLN:HB2	1.70	0.74
1:A:469:LYS:HG3	1:A:521:ILE:HG22	1.68	0.73
1:D:747:HIS:HD2	1:D:764:PHE:CD1	2.04	0.72
1:A:734:ARG:CZ	1:A:751:ARG:HH12	2.04	0.71
1:D:418:ASN:HD22	1:D:470:ASN:HD21	1.42	0.67
1:A:307:MET:HG2	1:A:747:HIS:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LYS:HG3	1:D:521:ILE:HG22	1.77	0.66
1:D:60:GLU:OE2	1:D:61:ASP:N	2.28	0.65
1:A:60:GLU:N	3:A:823:HOH:O	2.28	0.65
1:A:352:SER:HB3	1:A:355:ILE:HG22	1.78	0.65
1:A:734:ARG:NE	1:A:751:ARG:HH12	1.95	0.64
1:D:734:ARG:CZ	1:D:751:ARG:HH12	2.11	0.63
1:A:109:CYS:HB3	1:A:119:TRP:CZ3	2.35	0.62
1:D:109:CYS:HB3	1:D:119:TRP:CZ3	2.35	0.62
1:A:263:LEU:HD22	1:A:268:PHE:CD2	2.36	0.60
1:D:307:MET:HG2	1:D:747:HIS:CE1	2.36	0.60
1:A:772:TYR:OH	1:A:774:SER:HB3	2.02	0.59
1:D:528:THR:CG2	1:D:531:GLN:HB2	2.31	0.58
1:D:372:TRP:CZ2	1:D:384:GLY:HA3	2.39	0.58
1:D:734:ARG:NE	1:D:751:ARG:HH12	2.01	0.58
1:A:418:ASN:HD22	1:A:470:ASN:HD21	1.51	0.58
1:A:772:TYR:CZ	1:A:774:SER:HB3	2.40	0.57
1:A:307:MET:CG	1:A:747:HIS:CE1	2.88	0.57
1:D:109:CYS:HB3	1:D:119:TRP:CE3	2.40	0.56
1:D:772:TYR:OH	1:D:774:SER:HB3	2.05	0.56
1:A:352:SER:HB3	1:A:355:ILE:CG2	2.37	0.55
1:A:109:CYS:HB3	1:A:119:TRP:CE3	2.42	0.54
1:D:352:SER:HB3	1:D:355:ILE:HG22	1.88	0.54
1:D:445:ILE:HD11	1:D:457:PRO:HB3	1.89	0.54
1:D:263:LEU:HD22	1:D:268:PHE:CD2	2.43	0.54
1:A:734:ARG:NE	1:A:751:ARG:NH1	2.57	0.53
1:A:690:LYS:HE3	1:A:701:TYR:O	2.08	0.53
1:D:772:TYR:CZ	1:D:774:SER:HB3	2.43	0.53
1:D:70:LEU:HD23	1:D:71:ARG:N	2.24	0.53
1:D:22:LEU:HD22	1:D:133:TRP:CE2	2.44	0.52
1:A:22:LEU:HD22	1:A:133:TRP:CE2	2.44	0.52
1:A:314:THR:HG21	1:A:319:LEU:HD22	1.92	0.52
1:D:29:LEU:HD12	1:D:29:LEU:H	1.74	0.52
1:A:151:GLN:HE21	1:A:762:SER:HB2	1.75	0.51
1:A:313:LEU:HD12	1:A:314:THR:N	2.25	0.51
1:D:751:ARG:HD2	1:D:755:ASN:OD1	2.11	0.51
1:D:700:TYR:CE2	1:D:702:ASN:HB2	2.46	0.50
1:A:232:GLU:HG3	1:D:232:GLU:HG3	1.93	0.50
1:A:240:GLN:HG3	1:D:695:ASN:HD22	1.76	0.50
1:D:287:VAL:HG11	1:D:300:GLU:HB2	1.94	0.49
1:D:690:LYS:HE3	1:D:701:TYR:O	2.11	0.49
1:A:307:MET:CG	1:A:747:HIS:HE1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:LEU:HD11	1:D:94:PHE:CD2	2.47	0.49
1:A:11:ILE:HD12	1:A:11:ILE:N	2.27	0.48
1:D:307:MET:CG	1:D:747:HIS:CE1	2.96	0.48
1:A:445:ILE:HD11	1:A:457:PRO:HB3	1.94	0.48
1:D:314:THR:HG21	1:D:319:LEU:HD22	1.94	0.48
1:D:411:PRO:HG2	1:D:622:TYR:OH	2.13	0.48
1:D:370:ASP:HA	1:D:417:GLU:HB2	1.95	0.48
1:A:410:TYR:HB3	1:A:411:PRO:HD2	1.95	0.48
1:A:526:PHE:HB2	1:A:542:SER:OG	2.13	0.48
1:D:734:ARG:NE	1:D:751:ARG:NH1	2.62	0.48
1:A:151:GLN:NE2	1:A:762:SER:HB2	2.29	0.47
1:D:151:GLN:HE21	1:D:762:SER:CB	2.27	0.47
1:A:151:GLN:HE21	1:A:762:SER:CB	2.28	0.47
1:D:21:GLN:NE2	1:D:26:ASP:OD2	2.47	0.47
1:D:162:LEU:HD22	1:D:177:ILE:HG12	1.96	0.47
1:A:483:LEU:HD12	1:A:527:THR:HB	1.96	0.47
1:A:352:SER:CB	1:A:355:ILE:HG22	2.44	0.47
1:D:70:LEU:HD23	1:D:70:LEU:C	2.36	0.47
1:A:411:PRO:HG2	1:A:622:TYR:OH	2.15	0.47
1:A:331:ALA:HB1	1:A:630:ARG:HD3	1.98	0.46
1:A:659:ALA:HB3	1:A:699:PRO:HG2	1.97	0.46
1:A:29:LEU:HD12	1:A:29:LEU:H	1.81	0.46
1:D:264:HIS:ND1	1:D:267:LEU:HD12	2.30	0.46
1:D:411:PRO:HB3	1:D:462:LEU:O	2.14	0.46
1:A:360:LEU:HD13	1:A:404:ALA:HA	1.96	0.46
1:D:146:SER:O	1:D:149:LYS:HG2	2.16	0.46
1:A:236:LYS:HE3	1:D:227:GLU:OE1	2.16	0.46
1:D:410:TYR:HB3	1:D:411:PRO:HD2	1.97	0.46
1:A:287:VAL:HG11	1:A:300:GLU:HB2	1.97	0.46
1:D:151:GLN:HE21	1:D:762:SER:HB2	1.81	0.45
1:A:143:ASN:O	1:A:147:LEU:HD12	2.16	0.45
1:D:331:ALA:HB1	1:D:630:ARG:HD3	1.98	0.45
1:A:370:ASP:HA	1:A:417:GLU:HB2	1.99	0.45
1:A:734:ARG:CZ	1:A:751:ARG:NH1	2.77	0.45
1:D:29:LEU:HD11	1:D:94:PHE:CG	2.52	0.45
1:D:710:LYS:HE3	1:D:772:TYR:CE2	2.51	0.45
1:A:36:SER:HA	1:A:84:ASP:OD1	2.16	0.45
1:D:325:MET:O	1:D:459:PRO:HD2	2.17	0.45
1:D:313:LEU:C	1:D:313:LEU:HD12	2.36	0.44
1:D:347:LEU:HD11	1:D:578:VAL:HG12	1.99	0.44
1:A:61:ASP:HB3	1:A:62:SER:H	1.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD12	1:A:313:LEU:C	2.37	0.44
1:A:365:ARG:HG3	1:A:622:TYR:CE1	2.52	0.44
1:A:810:ALA:O	1:A:813:ASN:ND2	2.51	0.44
1:D:374:GLY:HA3	1:D:378:GLU:O	2.18	0.44
1:A:162:LEU:HD22	1:A:177:ILE:HG12	1.99	0.44
1:A:772:TYR:OH	1:A:774:SER:CB	2.64	0.44
1:A:335:ASN:HB3	1:A:364:CYS:HA	1.98	0.44
1:D:365:ARG:HG3	1:D:622:TYR:CE1	2.53	0.44
1:D:713:LEU:HD22	1:D:716:LEU:HD12	2.00	0.44
1:D:352:SER:HB3	1:D:355:ILE:CG2	2.48	0.43
1:D:313:LEU:HD12	1:D:314:THR:N	2.33	0.43
1:A:195:ILE:HG23	1:A:200:TRP:HB2	1.99	0.43
1:A:227:GLU:OE1	1:D:236:LYS:HE3	2.18	0.43
1:D:151:GLN:NE2	1:D:762:SER:HB2	2.33	0.43
1:A:56:ILE:H	1:A:56:ILE:HG13	1.65	0.43
1:D:552:LYS:NZ	3:D:816:HOH:O	2.51	0.43
1:A:29:LEU:HD11	1:A:94:PHE:CD2	2.53	0.43
1:A:751:ARG:HD2	1:A:755:ASN:OD1	2.19	0.43
1:D:248:VAL:HG13	1:D:251:ARG:NH2	2.33	0.43
1:A:411:PRO:HB3	1:A:462:LEU:O	2.19	0.43
1:A:808:PRO:HB3	1:D:777:PHE:HE2	1.84	0.42
1:A:72:ASP:OD1	1:A:73:ILE:N	2.52	0.42
1:A:129:VAL:O	1:A:130:ALA:C	2.58	0.42
1:D:687:PHE:CD2	1:D:706:PHE:CD2	3.08	0.42
1:D:612:GLY:HA3	1:D:735:LEU:HD22	2.02	0.42
1:D:50:TYR:CD2	1:D:157:LYS:HG3	2.55	0.42
1:D:195:ILE:HG23	1:D:200:TRP:HB2	2.01	0.42
1:A:307:MET:HG2	1:A:747:HIS:ND1	2.35	0.42
1:A:22:LEU:HD22	1:A:133:TRP:CZ2	2.54	0.42
1:A:287:VAL:HG11	1:A:300:GLU:CB	2.50	0.42
1:A:613:VAL:HG23	1:A:735:LEU:HD21	2.01	0.42
1:D:29:LEU:HD13	1:D:123:VAL:HB	2.01	0.42
1:A:681:ASP:HA	3:A:822:HOH:O	2.19	0.41
1:A:264:HIS:ND1	1:A:267:LEU:HD12	2.35	0.41
1:D:238:LEU:HD21	1:D:253:PHE:CD1	2.55	0.41
1:D:607:MET:HE3	1:D:611:LEU:HG	2.02	0.41
1:A:263:LEU:CD2	1:A:268:PHE:CD2	3.02	0.41
1:A:710:LYS:HE3	1:A:772:TYR:CE2	2.56	0.41
1:A:248:VAL:HG13	1:A:251:ARG:NH2	2.36	0.41
1:A:563:TYR:CE1	1:A:567:GLN:OE1	2.73	0.41
1:A:315:PRO:HG2	1:A:318:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:MET:CG	1:D:747:HIS:HE1	2.33	0.41
1:D:335:ASN:HB3	1:D:364:CYS:HA	2.02	0.41
1:D:775:ASP:O	1:D:777:PHE:HB2	2.20	0.41
1:A:60:GLU:HG3	1:A:61:ASP:CB	2.50	0.41
1:A:653:GLU:HB2	1:A:768:VAL:HB	2.03	0.40
1:D:557:PRO:HB2	1:D:638:PRO:HD2	2.03	0.40
1:A:499:LYS:HB3	1:A:499:LYS:HE3	1.95	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	775/813 (95%)	746 (96%)	26 (3%)	3 (0%)	34 69
1	D	767/813 (94%)	738 (96%)	28 (4%)	1 (0%)	51 83
All	All	1542/1626 (95%)	1484 (96%)	54 (4%)	4 (0%)	41 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	289	LYS
1	A	739	ASP
1	D	289	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	687/709 (97%)	653 (95%)	34 (5%)	25	61
1	D	684/709 (96%)	658 (96%)	26 (4%)	33	67
All	All	1371/1418 (97%)	1311 (96%)	60 (4%)	28	64

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	29	LEU
1	A	56	ILE
1	A	57	GLU
1	A	59	LYS
1	A	60	GLU
1	A	61	ASP
1	A	64	LEU
1	A	65	LEU
1	A	117	LEU
1	A	128	SER
1	A	185	LYS
1	A	189	THR
1	A	240	GLN
1	A	263	LEU
1	A	308	CYS
1	A	328	SER
1	A	373	ASP
1	A	375	LYS
1	A	409	GLU
1	A	422	VAL
1	A	472	LYS
1	A	492	LYS
1	A	503	THR
1	A	515	SER
1	A	528	THR
1	A	534	LYS
1	A	560	PHE
1	A	581	SER
1	A	645	ASP
1	A	713	LEU
1	A	737	PRO
1	A	775	ASP

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Mol	Chain	Res	Type
1	A	809	ASP
1	D	29	LEU
1	D	57	GLU
1	D	60	GLU
1	D	61	ASP
1	D	64	LEU
1	D	128	SER
1	D	185	LYS
1	D	189	THR
1	D	240	GLN
1	D	263	LEU
1	D	308	CYS
1	D	328	SER
1	D	373	ASP
1	D	409	GLU
1	D	422	VAL
1	D	472	LYS
1	D	474	HIS
1	D	503	THR
1	D	519	ASN
1	D	528	THR
1	D	560	PHE
1	D	581	SER
1	D	713	LEU
1	D	775	ASP
1	D	795	ASP
1	D	809	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	148	ASN
1	A	443	ASN
1	A	470	ASN
1	A	548	GLN
1	A	694	ASN
1	A	747	HIS
1	D	63	GLN
1	D	148	ASN
1	D	258	GLN
1	D	311	ASN

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Mol	Chain	Res	Type
1	D	418	ASN
1	D	443	ASN
1	D	531	GLN
1	D	548	GLN
1	D	694	ASN

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

Of 2 ligands modelled in this entry, 2 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

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	781/813 (96%)	-0.09	19 (2%)	59	44	38, 53, 74, 96	0
1	D	775/813 (95%)	0.13	31 (4%)	38	25	47, 68, 102, 131	0
All	All	1556/1626 (95%)	0.02	50 (3%)	47	31	38, 60, 93, 131	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	ASN	5.6
1	A	60	GLU	3.7
1	A	98	ASN	3.7
1	D	295	GLY	3.5
1	A	93	ASN	3.3
1	D	376	ASP	3.3
1	D	60	GLU	3.2
1	D	61	ASP	3.1
1	D	488	ASP	3.1
1	D	266	THR	3.0
1	A	534	LYS	2.9
1	D	264	HIS	2.8
1	D	645	ASP	2.8
1	D	57	GLU	2.8
1	D	486	LEU	2.7
1	A	57	GLU	2.7
1	D	97	SER	2.7
1	D	91	GLY	2.6
1	D	99	ILE	2.5
1	A	646	GLY	2.5
1	A	810	ALA	2.5
1	A	97	SER	2.5
1	A	92	THR	2.5
1	D	169	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	2.4
1	D	294	LYS	2.4
1	D	795	ASP	2.4
1	A	59	LYS	2.4
1	D	34	GLY	2.4
1	D	205	ASN	2.4
1	D	248	VAL	2.4
1	A	58	GLY	2.3
1	D	24	LYS	2.3
1	D	422	VAL	2.3
1	A	773	VAL	2.3
1	A	813	ASN	2.3
1	A	488	ASP	2.2
1	A	56	ILE	2.2
1	D	491	LYS	2.2
1	D	83	LYS	2.2
1	D	89	ASP	2.1
1	A	266	THR	2.1
1	D	487	THR	2.1
1	D	349	GLY	2.1
1	D	86	LYS	2.1
1	D	492	LYS	2.1
1	D	387	MET	2.1
1	A	61	ASP	2.1
1	A	96	SER	2.0
1	D	96	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	D	1000	1/1	0.91	0.15	74,74,74,74	0
2	CA	A	1000	1/1	0.93	0.16	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.