



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:06 AM UTC

PDB ID : 4J18 / pdb_00004j18
Title : Crystal structure of H191L mutant of UDP-glucose pyrophosphorylase from Leishmania major
Authors : Fuehring, J.I.; Routier, F.H.; Lamerz, A.-C.; Baruch, P.; Gerardy-Schahn, R.; Fedorov, R.
Deposited on : 2013-02-01
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

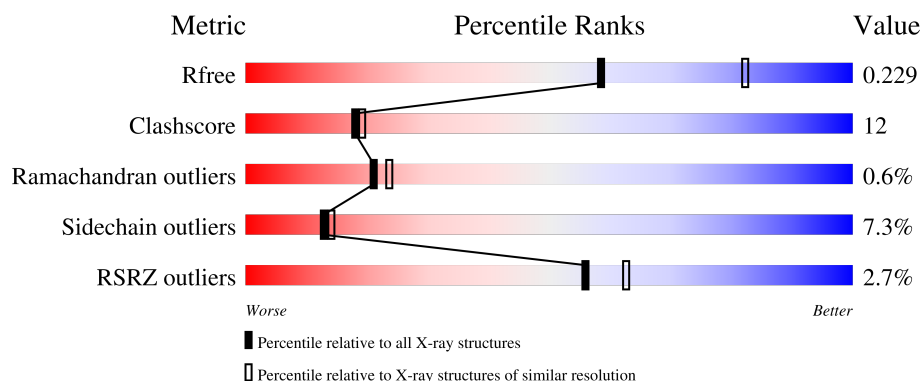
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	505	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4053 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 UDP-glucose pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	485	3744	2360	636	721	27	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	LEU	HIS	engineered mutation	UNP Q4QDU3
A	495	MET	-	expression tag	UNP Q4QDU3
A	496	ARG	-	expression tag	UNP Q4QDU3
A	497	PRO	-	expression tag	UNP Q4QDU3
A	498	LEU	-	expression tag	UNP Q4QDU3
A	499	GLU	-	expression tag	UNP Q4QDU3
A	500	HIS	-	expression tag	UNP Q4QDU3
A	501	HIS	-	expression tag	UNP Q4QDU3
A	502	HIS	-	expression tag	UNP Q4QDU3
A	503	HIS	-	expression tag	UNP Q4QDU3
A	504	HIS	-	expression tag	UNP Q4QDU3
A	505	HIS	-	expression tag	UNP Q4QDU3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	309	Total	O	0	0
			309	309		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	101.31Å 101.31Å 71.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.50 – 2.35 19.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.50-2.35) 99.2 (19.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.178 , 0.232 0.193 , 0.229	Depositor DCC
R_{free} test set	1511 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4053	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	2.06	90/3813 (2.4%)	1.22	25/5164 (0.5%)

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	2

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	VAL	C-O	-6.96	1.16	1.24
1	A	246	VAL	C-O	-6.94	1.16	1.23
1	A	36	HIS	C-O	-6.87	1.16	1.24
1	A	198	LEU	C-O	-6.78	1.16	1.24
1	A	314	LEU	C-O	-6.71	1.18	1.24
1	A	77	VAL	C-O	-6.68	1.17	1.24
1	A	217	VAL	C-O	-6.66	1.16	1.24
1	A	112	LEU	C-O	-6.60	1.16	1.24
1	A	134	ASN	C-O	-6.55	1.16	1.24
1	A	93	ASP	C-O	-6.54	1.16	1.23
1	A	369	ILE	C-O	-6.45	1.17	1.24
1	A	116	TYR	C-O	-6.31	1.16	1.24
1	A	375	ARG	C-O	-6.28	1.16	1.24
1	A	151	TYR	C-O	-6.13	1.17	1.24
1	A	150	LEU	C-O	-6.12	1.17	1.24
1	A	243	LEU	C-O	-6.10	1.17	1.24
1	A	313	ARG	C-O	-6.00	1.16	1.24
1	A	52	ILE	C-O	-5.99	1.17	1.23
1	A	242	PHE	C-O	-5.97	1.17	1.23
1	A	79	LEU	C-O	-5.96	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	MET	C-O	-5.93	1.16	1.24
1	A	125	LEU	C-O	-5.86	1.16	1.23
1	A	139	THR	C-O	-5.81	1.17	1.24
1	A	223	LEU	C-O	-5.76	1.16	1.24
1	A	130	MET	C-O	-5.75	1.17	1.24
1	A	304	PHE	C-O	-5.74	1.17	1.24
1	A	158	VAL	C-O	-5.73	1.17	1.24
1	A	122	SER	C-O	-5.72	1.17	1.23
1	A	58	LEU	C-O	-5.72	1.16	1.23
1	A	113	GLN	C-O	-5.71	1.17	1.24
1	A	115	GLN	C-O	-5.70	1.17	1.24
1	A	282	LEU	C-O	-5.69	1.17	1.24
1	A	108	ASP	C-O	-5.57	1.17	1.24
1	A	57	SER	C-O	-5.56	1.17	1.23
1	A	120	HIS	C-O	-5.56	1.17	1.24
1	A	159	GLU	C-O	-5.53	1.17	1.24
1	A	310	LEU	C-O	-5.52	1.17	1.24
1	A	306	ASN	C-O	-5.51	1.17	1.24
1	A	232	LEU	C-O	-5.48	1.17	1.24
1	A	121	CYS	C-O	-5.48	1.17	1.24
1	A	38	MET	C-O	-5.47	1.17	1.24
1	A	199	TYR	C-O	-5.47	1.17	1.24
1	A	233	ALA	C-O	-5.46	1.17	1.24
1	A	138	SER	C-O	-5.43	1.17	1.24
1	A	240	ILE	C-O	-5.40	1.17	1.24
1	A	245	GLU	C-O	-5.40	1.17	1.24
1	A	219	ASN	C-O	-5.38	1.17	1.23
1	A	29	ILE	C-O	-5.36	1.17	1.24
1	A	357	GLY	C-O	-5.36	1.17	1.23
1	A	15	CYS	C-O	-5.34	1.18	1.24
1	A	34	ALA	C-O	-5.33	1.17	1.24
1	A	76	THR	C-O	-5.33	1.17	1.24
1	A	55	VAL	C-O	-5.33	1.18	1.24
1	A	204	LEU	C-O	-5.32	1.17	1.24
1	A	214	TYR	C-O	-5.31	1.17	1.23
1	A	450	VAL	C-O	-5.30	1.18	1.23
1	A	16	VAL	C-O	-5.30	1.18	1.24
1	A	78	VAL	C-O	-5.29	1.18	1.24
1	A	321	MET	C-O	-5.29	1.17	1.24
1	A	23	LYS	N-CA	-5.29	1.40	1.46
1	A	142	PHE	C-O	-5.27	1.18	1.24
1	A	126	ARG	C-O	-5.27	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	PRO	C-O	-5.26	1.17	1.24
1	A	82	ASN	C-O	-5.25	1.16	1.23
1	A	248	ARG	C-O	-5.24	1.17	1.23
1	A	83	GLY	C-O	-5.24	1.17	1.23
1	A	194	ILE	C-O	-5.22	1.18	1.24
1	A	147	TYR	C-O	-5.21	1.18	1.24
1	A	231	VAL	C-O	-5.20	1.18	1.24
1	A	281	LEU	C-O	-5.20	1.17	1.23
1	A	423	MET	C-O	-5.19	1.17	1.23
1	A	355	ALA	C-O	-5.19	1.17	1.24
1	A	72	VAL	C-O	-5.14	1.18	1.24
1	A	235	MET	C-O	-5.14	1.18	1.24
1	A	347	PRO	N-CD	5.12	1.54	1.47
1	A	189	PRO	C-O	-5.11	1.17	1.24
1	A	195	TYR	C-O	-5.11	1.18	1.24
1	A	374	SER	C-O	-5.09	1.17	1.24
1	A	290	LYS	C-O	-5.07	1.18	1.24
1	A	228	ASP	C-O	-5.07	1.18	1.24
1	A	307	THR	C-O	-5.06	1.17	1.24
1	A	473	PHE	C-O	-5.06	1.17	1.24
1	A	54	PRO	C-O	-5.05	1.17	1.23
1	A	127	PHE	C-O	-5.05	1.18	1.24
1	A	224	GLY	C-O	-5.04	1.17	1.24
1	A	457	VAL	C-O	-5.04	1.18	1.24
1	A	359	ALA	C-O	-5.03	1.17	1.24
1	A	279	VAL	C-O	-5.01	1.18	1.24
1	A	148	PRO	C-O	-5.00	1.18	1.24
1	A	211	GLY	C-O	-5.00	1.17	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	VAL	N-CA-C	10.21	120.13	110.53
1	A	84	GLY	N-CA-C	9.05	123.82	112.14
1	A	22	ALA	N-CA-C	8.42	122.86	112.59
1	A	191	LEU	N-CA-C	7.31	120.11	111.71
1	A	293	MET	N-CA-C	7.26	119.20	111.28
1	A	284	GLU	CB-CA-C	-6.75	98.35	110.36
1	A	145	ALA	N-CA-C	6.74	118.42	111.14
1	A	203	LYS	N-CA-C	6.58	118.53	111.36
1	A	346	SER	CA-C-N	-6.24	113.33	119.76
1	A	346	SER	C-N-CA	-6.24	113.33	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	PRO	N-CA-C	6.18	125.20	112.47
1	A	82	ASN	CA-C-N	6.16	126.77	120.00
1	A	82	ASN	C-N-CA	6.16	126.77	120.00
1	A	56	ASP	N-CA-C	6.11	117.74	111.14
1	A	257	GLY	N-CA-C	6.11	119.58	111.03
1	A	269	LYS	CB-CA-C	-6.03	98.64	110.10
1	A	122	SER	N-CA-C	6.03	117.45	107.20
1	A	273	PRO	CA-N-CD	-5.80	103.88	112.00
1	A	159	GLU	N-CA-C	5.69	118.81	109.76
1	A	7	SER	CB-CA-C	-5.46	99.72	110.10
1	A	442	LYS	N-CA-C	5.33	116.90	111.14
1	A	488	PRO	CA-N-CD	-5.32	104.56	112.00
1	A	307	THR	N-CA-C	5.18	117.83	111.82
1	A	83	GLY	N-CA-C	5.13	119.34	112.77
1	A	431	VAL	N-CA-C	5.07	116.42	111.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	PRO	Peptide
1	A	22	ALA	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	3744	0	3737	91	0
2	A	309	0	0	21	0
All	All	4053	0	3737	91	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 12.

All (91) 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:268:GLY:HA2	1:A:269:LYS:CB	1.53	1.35
1:A:268:GLY:CA	1:A:269:LYS:HB2	1.62	1.23
1:A:249:ARG:HG2	1:A:305:PHE:HB2	1.33	1.03
1:A:351:GLN:HB3	2:A:1279:HOH:O	1.59	1.00
1:A:271:GLY:C	1:A:273:PRO:HD3	2.00	0.85
1:A:339:VAL:HG12	1:A:346:SER:HB2	1.59	0.84
1:A:268:GLY:HA2	1:A:269:LYS:HB2	0.83	0.83
1:A:5:MET:O	1:A:7:SER:HB3	1.80	0.80
1:A:152:GLN:HG2	2:A:1266:HOH:O	1.84	0.77
1:A:284:GLU:H	1:A:287:GLN:HE21	1.32	0.77
1:A:267:LYS:O	1:A:269:LYS:HB2	1.85	0.76
1:A:167:LYS:HE3	1:A:184:TYR:O	1.86	0.76
1:A:133:PHE:CE2	2:A:1092:HOH:O	2.41	0.73
1:A:267:LYS:O	1:A:269:LYS:HG3	1.88	0.73
1:A:249:ARG:CG	1:A:305:PHE:HB2	2.15	0.73
1:A:149:TRP:HB2	2:A:1108:HOH:O	1.91	0.70
1:A:6:LYS:HA	1:A:8:LEU:N	2.09	0.67
1:A:144:LYS:HB2	1:A:151:TYR:CD1	2.29	0.67
1:A:475:ILE:HG23	1:A:476:PRO:HD2	1.75	0.67
1:A:74:GLN:OE1	1:A:122:SER:HB2	1.95	0.67
1:A:305:PHE:CD1	2:A:1240:HOH:O	2.46	0.67
1:A:213:ARG:NH2	1:A:236:GLU:OE1	2.25	0.66
1:A:351:GLN:CG	2:A:1279:HOH:O	2.43	0.66
1:A:459:THR:HB	1:A:482:ASN:HD22	1.61	0.65
1:A:167:LYS:HD3	1:A:351:GLN:NE2	2.12	0.65
1:A:268:GLY:HA2	1:A:269:LYS:HB3	1.69	0.65
1:A:268:GLY:CA	1:A:269:LYS:CB	2.40	0.64
1:A:334:ARG:NH1	2:A:1009:HOH:O	2.28	0.64
1:A:169:LEU:HD12	1:A:174:GLU:HG2	1.79	0.63
1:A:7:SER:O	1:A:7:SER:OG	2.14	0.63
1:A:149:TRP:HE3	2:A:1108:HOH:O	1.82	0.62
1:A:351:GLN:HG2	2:A:1279:HOH:O	1.99	0.62
1:A:475:ILE:CG2	1:A:476:PRO:HD2	2.29	0.62
1:A:249:ARG:HG2	1:A:305:PHE:CB	2.21	0.61
1:A:395:VAL:HG22	1:A:401:LEU:CD2	2.32	0.60
1:A:270:ASP:O	1:A:270:ASP:CG	2.45	0.59
1:A:284:GLU:H	1:A:287:GLN:NE2	1.99	0.59
1:A:98:LEU:HD23	1:A:106:PHE:HE1	1.68	0.59
1:A:290:LYS:HD2	2:A:1184:HOH:O	2.01	0.59
1:A:6:LYS:HA	1:A:7:SER:C	2.28	0.58
1:A:267:LYS:O	1:A:269:LYS:CG	2.51	0.58
1:A:144:LYS:HB2	1:A:151:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HB2	2:A:1278:HOH:O	2.02	0.57
1:A:100:VAL:O	1:A:389:ARG:HG2	2.05	0.57
1:A:267:LYS:O	1:A:269:LYS:CB	2.53	0.56
1:A:351:GLN:CB	2:A:1279:HOH:O	2.31	0.55
1:A:415:ASP:HB3	1:A:445:THR:HG23	1.88	0.55
1:A:98:LEU:HD23	1:A:106:PHE:CE1	2.42	0.54
1:A:149:TRP:CD1	1:A:149:TRP:H	2.25	0.53
1:A:459:THR:HB	1:A:482:ASN:ND2	2.24	0.52
1:A:74:GLN:HG2	2:A:1225:HOH:O	2.08	0.52
1:A:467:THR:HG22	2:A:1236:HOH:O	2.10	0.52
1:A:79:LEU:HD12	1:A:80:LYS:N	2.25	0.51
1:A:271:GLY:CA	1:A:273:PRO:HD3	2.40	0.51
1:A:461:THR:O	1:A:483:ASP:HA	2.10	0.51
1:A:191:LEU:HB2	2:A:1182:HOH:O	2.12	0.50
1:A:267:LYS:C	1:A:269:LYS:HB2	2.37	0.50
1:A:153:VAL:HB	1:A:157:GLU:HB2	1.92	0.49
1:A:74:GLN:CG	2:A:1225:HOH:O	2.61	0.48
1:A:178:TRP:HZ3	1:A:347:PRO:HD3	1.79	0.48
1:A:74:GLN:OE1	1:A:122:SER:CB	2.62	0.47
1:A:33:ILE:O	1:A:37:VAL:HG23	2.15	0.47
1:A:81:LEU:HD11	1:A:356:MET:SD	2.55	0.46
1:A:270:ASP:O	1:A:270:ASP:OD2	2.34	0.46
1:A:133:PHE:CD2	2:A:1092:HOH:O	2.64	0.46
1:A:235:MET:HG2	1:A:240:ILE:HB	1.97	0.46
1:A:395:VAL:HG22	1:A:401:LEU:HD21	1.96	0.45
1:A:457:VAL:C	1:A:458:LEU:HD12	2.42	0.45
1:A:271:GLY:C	1:A:273:PRO:CD	2.82	0.45
1:A:482:ASN:OD1	1:A:483:ASP:HB2	2.17	0.45
1:A:25:ASN:ND2	1:A:27:ALA:H	2.15	0.44
1:A:6:LYS:HA	1:A:8:LEU:H	1.81	0.44
1:A:65:THR:HG23	2:A:1111:HOH:O	2.17	0.44
1:A:267:LYS:HG2	1:A:268:GLY:N	2.32	0.44
1:A:90:GLY:HA2	1:A:423:MET:HE2	1.99	0.44
1:A:271:GLY:HA3	1:A:273:PRO:HD3	1.99	0.43
1:A:343:ASN:O	1:A:346:SER:OG	2.34	0.43
1:A:188:PRO:HA	1:A:189:PRO:HD3	1.76	0.43
1:A:116:TYR:HA	2:A:1063:HOH:O	2.18	0.43
1:A:170:GLN:HG2	1:A:350:TYR:CZ	2.54	0.42
1:A:251:GLU:HB3	2:A:1306:HOH:O	2.19	0.42
1:A:415:ASP:HB3	1:A:445:THR:HA	2.00	0.42
1:A:482:ASN:C	1:A:484:THR:HG22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:O	1:A:185:GLU:HG2	2.21	0.41
1:A:404:ASP:OD1	1:A:405:ASP:N	2.53	0.41
1:A:182:PRO:O	1:A:185:GLU:HB2	2.21	0.41
1:A:287:GLN:NE2	2:A:1101:HOH:O	2.51	0.41
1:A:167:LYS:HD3	1:A:351:GLN:HE21	1.85	0.40
1:A:458:LEU:N	1:A:458:LEU:CD1	2.84	0.40
1:A:453:GLY:H	1:A:456:ASN:ND2	2.19	0.40
1:A:482:ASN:O	1:A:484:THR:HG22	2.20	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	483/505 (96%)	473 (98%)	7 (1%)	3 (1%)	21	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	273	PRO
1	A	189	PRO

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	412/432 (95%)	382 (93%)	30 (7%)	13 14

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	6	LYS
1	A	17	LYS
1	A	23	LYS
1	A	49	ASP
1	A	73	LEU
1	A	74	GLN
1	A	79	LEU
1	A	98	LEU
1	A	118	ARG
1	A	130	MET
1	A	138	SER
1	A	141	SER
1	A	194	ILE
1	A	237	LYS
1	A	251	GLU
1	A	266	VAL
1	A	267	LYS
1	A	269	LYS
1	A	284	GLU
1	A	301	LYS
1	A	337	LYS
1	A	341	SER
1	A	346	SER
1	A	351	GLN
1	A	367	SER
1	A	380	LYS
1	A	403	LEU
1	A	440	GLU
1	A	484	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	25	ASN
1	A	113	GLN

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Mol	Chain	Res	Type
1	A	115	GLN
1	A	120	HIS
1	A	170	GLN
1	A	210	GLN
1	A	219	ASN
1	A	287	GLN
1	A	309	ASN
1	A	322	GLN
1	A	351	GLN
1	A	451	GLN
1	A	456	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	485/505 (96%)	-0.03	13 (2%) 56 63	16, 33, 62, 120	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ASP	6.8
1	A	271	GLY	5.0
1	A	269	LYS	4.9
1	A	5	MET	4.3
1	A	4	ASP	3.7
1	A	273	PRO	3.7
1	A	275	ALA	3.2
1	A	272	GLN	3.0
1	A	7	SER	2.7
1	A	410	HIS	2.4
1	A	488	PRO	2.4
1	A	179	ALA	2.4
1	A	482	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.