



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:21 AM UTC

PDB ID : 5JXK / pdb_00005jxk
Title : Crystal structure of Porphyromonas endodontalis DPP11
Authors : Bezerra, G.A.; Cornaciu, I.; Hoffmann, G.; Djinovic-Carugo, K.; Marquez, J.A.
Deposited on : 2016-05-13
Resolution : 2.85 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

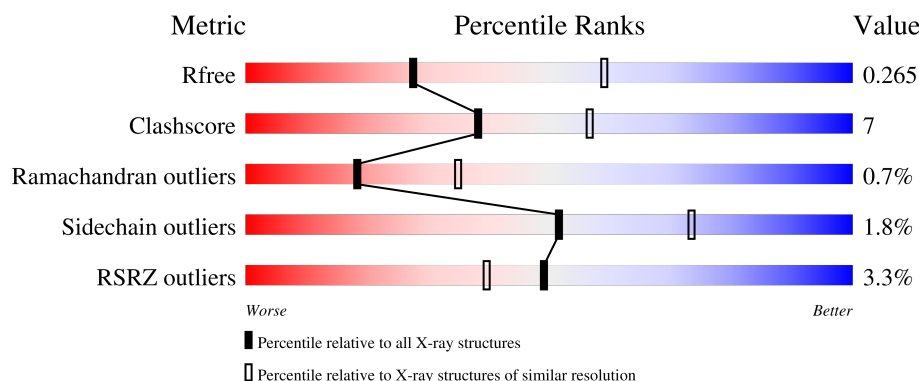
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	703	2% 83% 15% .
1	B	703	4% 77% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10799 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 Asp/Glu-specific dipeptidyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	1	0
			5451	3453	945	1029	24			
1	B	681	Total	C	N	O	S	0	0	0
			5293	3356	905	1007	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP F8WQK8
A	652	ALA	SER	engineered mutation	UNP F8WQK8
A	718	HIS	-	expression tag	UNP F8WQK8
A	719	HIS	-	expression tag	UNP F8WQK8
A	720	HIS	-	expression tag	UNP F8WQK8
A	721	HIS	-	expression tag	UNP F8WQK8
A	722	HIS	-	expression tag	UNP F8WQK8
A	723	HIS	-	expression tag	UNP F8WQK8
B	21	MET	-	initiating methionine	UNP F8WQK8
B	652	ALA	SER	engineered mutation	UNP F8WQK8
B	718	HIS	-	expression tag	UNP F8WQK8
B	719	HIS	-	expression tag	UNP F8WQK8
B	720	HIS	-	expression tag	UNP F8WQK8
B	721	HIS	-	expression tag	UNP F8WQK8
B	722	HIS	-	expression tag	UNP F8WQK8
B	723	HIS	-	expression tag	UNP F8WQK8

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	1	Total	Cl	0	0
			1	1		

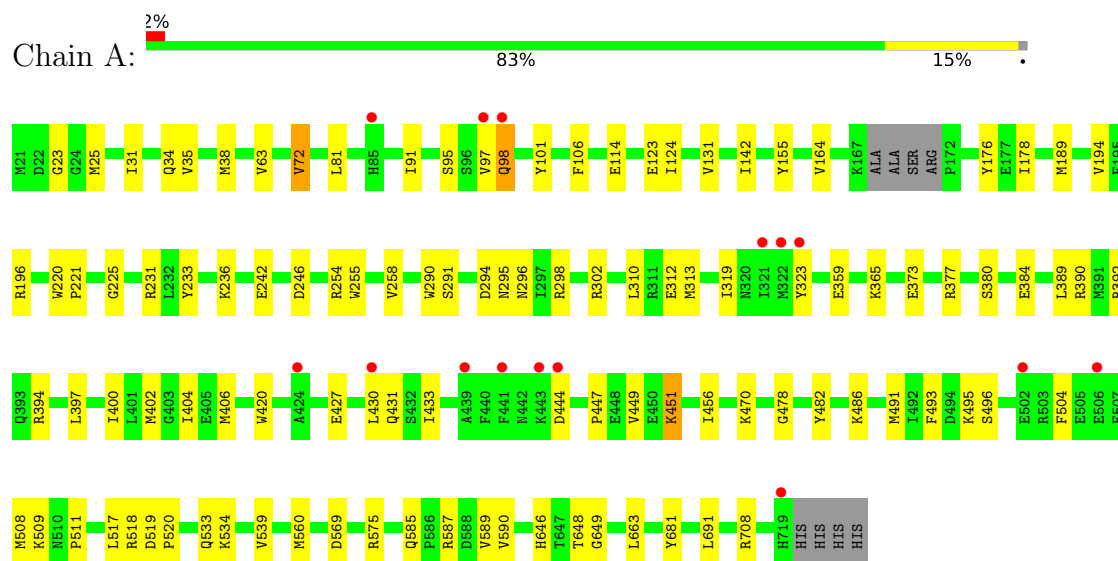
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	17	Total 17	O 17	0	0

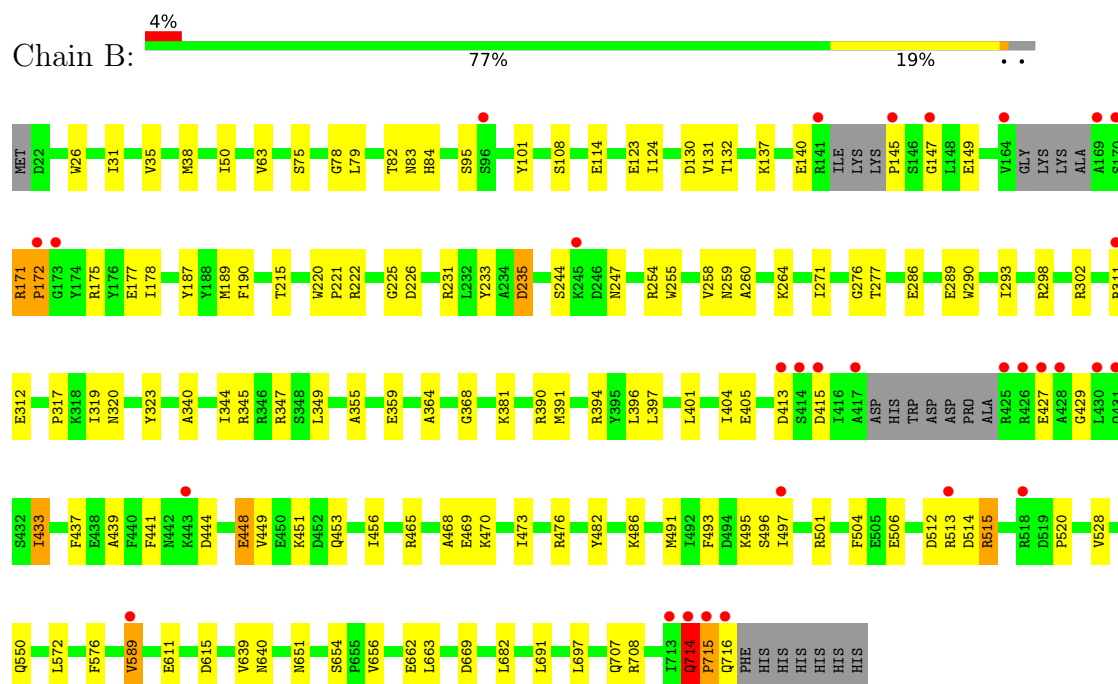
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Asp/Glu-specific dipeptidyl-peptidase



• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.75Å 91.83Å 229.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.85 46.70 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.70-2.85) 100.0 (46.70-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.273 0.239 , 0.265	Depositor DCC
R_{free} test set	1944 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 20.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10799	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

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

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	0.30	0/5575	0.73	4/7546 (0.1%)
1	B	0.31	0/5404	0.78	8/7316 (0.1%)
All	All	0.31	0/10979	0.76	12/14862 (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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	714	GLN	CA-C-N	-8.75	108.90	119.84
1	B	714	GLN	C-N-CA	-8.75	108.90	119.84
1	A	431	GLN	N-CA-C	-6.64	104.65	112.89
1	A	519	ASP	CA-C-N	5.71	125.18	119.24
1	A	519	ASP	C-N-CA	5.71	125.18	119.24
1	B	404	ILE	CA-C-N	5.44	127.57	120.28
1	B	404	ILE	C-N-CA	5.44	127.57	120.28
1	B	682	LEU	CA-C-N	5.39	124.58	118.97
1	B	682	LEU	C-N-CA	5.39	124.58	118.97
1	B	615	ASP	CA-C-N	5.35	125.42	119.32
1	B	615	ASP	C-N-CA	5.35	125.42	119.32
1	A	98	GLN	N-CA-C	-5.16	107.02	113.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	ASP	Peptide

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	5451	0	5258	62	0
1	B	5293	0	5087	85	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	35	0	0	1	0
3	B	17	0	0	3	0
All	All	10799	0	10345	146	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 7.

All (146) 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:B:132:THR:HG22	1:B:187:TYR:H	1.42	0.81
1:B:390:ARG:HH21	1:B:394:ARG:HH21	1.27	0.81
1:B:75:SER:OG	1:B:78:GLY:N	2.21	0.74
1:B:405:GLU:H	1:B:405:GLU:CD	1.96	0.73
1:B:171:ARG:H	1:B:172:PRO:HD3	1.55	0.72
1:B:222:ARG:NH1	1:B:669:ASP:OD2	2.23	0.71
1:B:254:ARG:NH1	1:B:255:TRP:O	2.25	0.69
1:A:35:VAL:HA	1:A:38:MET:HE2	1.74	0.68
1:B:415:ASP:HB2	1:B:427:GLU:HG3	1.75	0.67
1:A:25:MET:HE3	1:A:646:HIS:CD2	2.33	0.64
1:B:515:ARG:HH11	1:B:515:ARG:HG3	1.62	0.64
1:A:496:SER:HB2	1:A:520:PRO:HG2	1.80	0.62
1:A:389:LEU:HB3	1:A:539:VAL:HG22	1.82	0.62
1:A:114:GLU:OE2	1:A:708:ARG:NH2	2.33	0.61
1:A:359:GLU:HG2	1:A:560:MET:HE1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ARG:NH2	3:B:904:HOH:O	2.32	0.61
1:B:469:GLU:HG3	1:B:470:LYS:HG3	1.84	0.59
1:B:95:SER:OG	1:B:101:TYR:N	2.36	0.59
1:A:447:PRO:O	1:A:451:LYS:HG3	2.04	0.58
1:B:298:ARG:HG3	1:B:302:ARG:HD2	1.87	0.57
1:B:276:GLY:HA2	1:B:572:LEU:HG	1.87	0.57
1:A:236:LYS:NZ	1:A:246:ASP:O	2.37	0.57
1:A:451:LYS:HG2	1:A:493:PHE:CG	2.40	0.56
1:B:497:ILE:HG22	1:B:504:PHE:HA	1.88	0.56
1:A:294:ASP:O	1:A:394:ARG:NH2	2.39	0.56
1:A:569:ASP:O	1:A:575:ARG:NH2	2.36	0.56
1:B:413:ASP:OD2	1:B:429:GLY:HA3	2.05	0.56
1:B:131:VAL:HG11	1:B:189:MET:HE3	1.89	0.55
1:B:482:TYR:CZ	1:B:491:MET:HG3	2.41	0.55
1:A:380:SER:O	1:A:384:GLU:HG3	2.07	0.55
1:A:63:VAL:HG12	1:A:124:ILE:HG12	1.89	0.55
1:B:496:SER:HB2	1:B:520:PRO:HG2	1.88	0.54
1:A:298:ARG:HG3	1:A:302:ARG:HD2	1.88	0.54
1:B:177:GLU:HB3	1:B:190:PHE:HB2	1.90	0.54
1:B:264:LYS:NZ	3:B:903:HOH:O	2.32	0.54
1:B:114:GLU:OE2	1:B:708:ARG:NH2	2.37	0.54
1:B:235:ASP:N	1:B:235:ASP:OD1	2.40	0.54
1:A:400:ILE:HG23	1:A:404:ILE:HD12	1.89	0.54
1:B:31:ILE:HD11	1:B:50:ILE:HD12	1.90	0.54
1:A:587:ARG:NH1	3:A:904:HOH:O	2.39	0.53
1:B:220:TRP:CD2	1:B:221:PRO:HA	2.43	0.53
1:A:392:ARG:HD3	1:A:470:LYS:HB3	1.90	0.53
1:A:123:GLU:HG2	1:A:194:VAL:HG12	1.91	0.53
1:B:178:ILE:HD11	1:B:189:MET:HE2	1.91	0.53
1:B:451:LYS:HE3	1:B:493:PHE:CD1	2.44	0.53
1:B:465:ARG:NH2	3:B:905:HOH:O	2.42	0.52
1:A:91:ILE:O	1:A:95:SER:OG	2.25	0.52
1:B:258:VAL:HG22	1:B:663:LEU:HD23	1.92	0.52
1:B:396:LEU:HD11	1:B:528:VAL:HG13	1.92	0.52
1:A:220:TRP:CD2	1:A:221:PRO:HA	2.45	0.52
1:B:355:ALA:O	1:B:359:GLU:HG3	2.10	0.52
1:A:221:PRO:HB3	1:B:589:VAL:HB	1.91	0.52
1:B:260:ALA:H	1:B:716:GLN:H	1.58	0.52
1:A:196:ARG:HB2	1:A:242:GLU:HA	1.92	0.52
1:A:254:ARG:NH1	1:A:255:TRP:O	2.44	0.51
1:B:171:ARG:H	1:B:172:PRO:CD	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG12	1:B:124:ILE:HG12	1.93	0.51
1:A:101:TYR:HB3	1:A:106:PHE:HB2	1.93	0.51
1:A:397:LEU:HG	1:A:402:MET:HE2	1.94	0.50
1:A:456:ILE:HD13	1:A:486:LYS:HG3	1.94	0.50
1:B:317:PRO:O	1:B:320:ASN:N	2.44	0.50
1:B:319:ILE:HG23	1:B:323:TYR:CD2	2.47	0.50
1:B:512:ASP:OD1	1:B:513:ARG:N	2.44	0.50
1:B:512:ASP:OD1	1:B:514:ASP:N	2.45	0.50
1:A:131:VAL:HG11	1:A:189:MET:HE3	1.95	0.49
1:B:231:ARG:HD2	1:B:233:TYR:HE1	1.78	0.49
1:A:478:GLY:O	1:A:482:TYR:HD2	1.95	0.49
1:A:97:VAL:HG23	1:A:98:GLN:N	2.28	0.49
1:B:75:SER:CB	1:B:79:LEU:H	2.25	0.49
1:B:123:GLU:OE2	1:B:175:ARG:NH1	2.46	0.49
1:B:437:PHE:C	1:B:439:ALA:H	2.20	0.49
1:A:420:TRP:HH2	1:A:511:PRO:HB2	1.77	0.49
1:B:347:ARG:HH11	1:B:347:ARG:HG2	1.78	0.49
1:B:244:SER:N	1:B:247:ASN:OD1	2.45	0.48
1:A:517:LEU:HB3	1:A:518:ARG:NH1	2.28	0.48
1:B:397:LEU:HA	1:B:401:LEU:HB2	1.95	0.48
1:B:289:GLU:HG3	1:B:293:ILE:HD12	1.95	0.48
1:A:178:ILE:HD11	1:A:189:MET:HE2	1.96	0.47
1:A:298:ARG:HE	1:A:302:ARG:NH1	2.12	0.47
1:A:319:ILE:HG23	1:A:323:TYR:HD2	1.79	0.47
1:A:585:GLN:HG3	1:A:590:VAL:O	2.15	0.47
1:B:108:SER:O	1:B:708:ARG:NH1	2.41	0.47
1:B:640:ASN:ND2	1:B:691:LEU:HA	2.30	0.47
1:B:271:ILE:HG12	1:B:656:VAL:HG22	1.97	0.47
1:A:404:ILE:HG22	1:A:406:MET:H	1.80	0.47
1:B:344:ILE:HD13	1:B:349:LEU:HB3	1.97	0.47
1:A:225:GLY:HA2	1:A:691:LEU:HD13	1.97	0.46
1:B:433:ILE:H	1:B:433:ILE:HG13	1.55	0.46
1:B:456:ILE:HD13	1:B:486:LYS:HG3	1.98	0.46
1:B:697:LEU:HD13	1:B:715:PRO:HB3	1.97	0.46
1:A:258:VAL:HG22	1:A:663:LEU:HD23	1.97	0.46
1:A:648:THR:OG1	1:A:649:GLY:N	2.48	0.45
1:B:427:GLU:OE1	1:B:427:GLU:HA	2.16	0.45
1:B:35:VAL:HA	1:B:38:MET:HE3	1.97	0.45
1:B:215:THR:N	1:B:611:GLU:OE2	2.46	0.45
1:B:84:HIS:N	1:B:226:ASP:OD1	2.44	0.45
1:B:108:SER:OG	1:B:708:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ASP:CG	1:B:429:GLY:HA3	2.42	0.45
1:B:640:ASN:HD22	1:B:691:LEU:HA	1.82	0.45
1:B:415:ASP:OD2	1:B:427:GLU:HB3	2.15	0.45
1:B:651:ASN:O	1:B:654:SER:OG	2.34	0.45
1:A:646:HIS:ND1	1:A:681:TYR:HB2	2.32	0.44
1:A:294:ASP:OD1	1:A:390:ARG:NH1	2.50	0.44
1:B:468:ALA:O	1:B:476:ARG:HG3	2.17	0.44
1:A:646:HIS:CE1	1:A:681:TYR:HB2	2.52	0.44
1:B:364:ALA:O	1:B:368:GLY:N	2.51	0.44
1:B:415:ASP:OD1	1:B:415:ASP:N	2.43	0.44
1:A:23:GLY:HA3	1:A:681:TYR:CD2	2.52	0.44
1:A:97:VAL:HG23	1:A:98:GLN:H	1.83	0.44
1:B:319:ILE:HD11	1:B:448:GLU:OE1	2.17	0.44
1:A:34:GLN:O	1:A:38:MET:HG3	2.18	0.44
1:B:347:ARG:HG2	1:B:347:ARG:NH1	2.32	0.44
1:B:312:GLU:HG2	1:B:449:VAL:HG12	2.00	0.43
1:A:365:LYS:HE2	1:A:365:LYS:HB3	1.83	0.43
1:A:25:MET:HE3	1:A:646:HIS:HD2	1.81	0.43
1:B:495:LYS:HD2	1:B:495:LYS:HA	1.79	0.43
1:A:533:GLN:HG3	1:A:534:LYS:N	2.34	0.43
1:B:441:PHE:CZ	1:B:501:ARG:HG2	2.54	0.43
1:A:310:LEU:HA	1:A:313:MET:HE2	2.00	0.43
1:A:430:LEU:HA	1:A:433:ILE:HB	1.99	0.43
1:B:130:ASP:OD1	1:B:132:THR:HG23	2.19	0.43
1:B:79:LEU:HD13	1:B:231:ARG:NH2	2.34	0.42
1:A:290:TRP:O	1:A:295:ASN:ND2	2.43	0.42
1:B:589:VAL:O	1:B:589:VAL:HG12	2.19	0.42
1:A:430:LEU:O	1:A:433:ILE:HG22	2.20	0.42
1:A:491:MET:HG3	1:A:495:LYS:HE2	2.02	0.42
1:A:312:GLU:HG3	1:A:449:VAL:HG13	2.02	0.42
1:A:491:MET:HE2	1:A:520:PRO:HB3	2.02	0.42
1:A:504:PHE:O	1:A:508:MET:HG2	2.20	0.42
1:B:75:SER:HB3	1:B:79:LEU:H	1.84	0.42
1:B:298:ARG:O	1:B:302:ARG:HB2	2.19	0.42
1:B:259:ASN:ND2	1:B:662:GLU:OE1	2.42	0.42
1:A:72:VAL:HG13	1:A:81:LEU:HB2	2.02	0.42
1:B:26:TRP:HB2	1:B:576:PHE:CE1	2.55	0.42
1:A:231:ARG:HD2	1:A:233:TYR:CE1	2.55	0.41
1:B:82:THR:OG1	1:B:83:ASN:N	2.49	0.41
1:B:145:PRO:C	1:B:147:GLY:H	2.28	0.41
1:B:290:TRP:CH2	1:B:340:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:HB2	1:B:427:GLU:CG	2.48	0.41
1:B:639:VAL:O	1:B:640:ASN:ND2	2.54	0.41
1:B:286:GLU:OE2	1:B:550:GLN:NE2	2.54	0.41
1:A:291:SER:O	1:A:296:ASN:ND2	2.40	0.40
1:A:31:ILE:HD11	1:A:38:MET:HE1	2.02	0.40
1:A:164:VAL:HG11	1:A:176:TYR:CE2	2.56	0.40
1:A:142:ILE:HD11	1:A:155:TYR:OH	2.21	0.40
1:B:225:GLY:HA2	1:B:691:LEU:HD13	2.02	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	692/703 (98%)	657 (95%)	34 (5%)	1 (0%)	48	68
1	B	673/703 (96%)	620 (92%)	45 (7%)	8 (1%)	10	22
All	All	1365/1406 (97%)	1277 (94%)	79 (6%)	9 (1%)	18	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	VAL
1	B	171	ARG
1	B	589	VAL
1	B	172	PRO
1	B	444	ASP
1	B	448	GLU
1	B	453	GLN
1	B	714	GLN
1	B	715	PRO

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	553/583 (95%)	547 (99%)	6 (1%)	65	81
1	B	534/583 (92%)	520 (97%)	14 (3%)	40	65
All	All	1087/1166 (93%)	1067 (98%)	20 (2%)	51	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	A	373	GLU
1	A	377	ARG
1	A	427	GLU
1	A	451	LYS
1	A	509	LYS
1	B	137	LYS
1	B	140	GLU
1	B	149	GLU
1	B	235	ASP
1	B	277	THR
1	B	311	ARG
1	B	381	LYS
1	B	391	MET
1	B	433	ILE
1	B	473	ILE
1	B	506	GLU
1	B	515	ARG
1	B	707	GLN
1	B	714	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	419	HIS

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Mol	Chain	Res	Type
1	A	453	GLN
1	A	640	ASN
1	A	651	ASN
1	B	85	HIS
1	B	565	ASN
1	B	640	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](#)

Of 3 ligands modelled in this entry, 3 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 ⓘ

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	695/703 (98%)	0.02	15 (2%) 62 53	13, 35, 73, 104	1 (0%)
1	B	681/703 (96%)	0.39	30 (4%) 39 30	17, 52, 95, 144	0
All	All	1376/1406 (97%)	0.20	45 (3%) 49 40	13, 44, 88, 144	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	ARG	4.9
1	A	85[A]	HIS	4.7
1	B	169	ALA	4.5
1	B	413	ASP	4.4
1	A	444	ASP	4.2
1	A	439	ALA	3.9
1	A	98	GLN	3.8
1	B	170	SER	3.8
1	B	425	ARG	3.6
1	B	145	PRO	3.6
1	B	716	GLN	3.4
1	B	417	ALA	3.4
1	B	428	ALA	3.4
1	A	323	TYR	3.0
1	B	173	GLY	3.0
1	A	321	ILE	2.9
1	A	441	PHE	2.7
1	A	322	MET	2.7
1	B	715	PRO	2.6
1	B	141	ARG	2.6
1	B	164	VAL	2.6
1	A	443	LYS	2.6
1	B	172	PRO	2.5
1	B	147	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	502	GLU	2.5
1	B	713	ILE	2.4
1	A	719	HIS	2.4
1	B	513	ARG	2.4
1	B	443	LYS	2.3
1	A	97	VAL	2.3
1	B	714	GLN	2.3
1	B	311	ARG	2.3
1	B	430	LEU	2.2
1	B	415	ASP	2.2
1	A	424	ALA	2.2
1	B	589	VAL	2.2
1	B	427	GLU	2.2
1	B	518	ARG	2.1
1	B	497	ILE	2.1
1	A	506	GLU	2.1
1	B	96	SER	2.0
1	B	431	GLN	2.0
1	B	414	SER	2.0
1	A	430	LEU	2.0
1	B	245	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CL	A	801	1/1	0.95	0.04	12,12,12,12	0
2	CL	A	802	1/1	0.97	0.13	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	801	1/1	0.97	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.