



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:10 AM UTC

PDB ID : 5JWI / pdb_00005jwi
Title : Crystal structure of Porphyromonas endodontalis DPP11 in complex with dipeptide Arg-Glu
Authors : Bezerra, G.A.; Fedosyuk, S.; Ohara-Nemoto, Y.; Nemoto, T.K.; Djcinovic-Carugo, K.
Deposited on : 2016-05-12
Resolution : 2.10 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

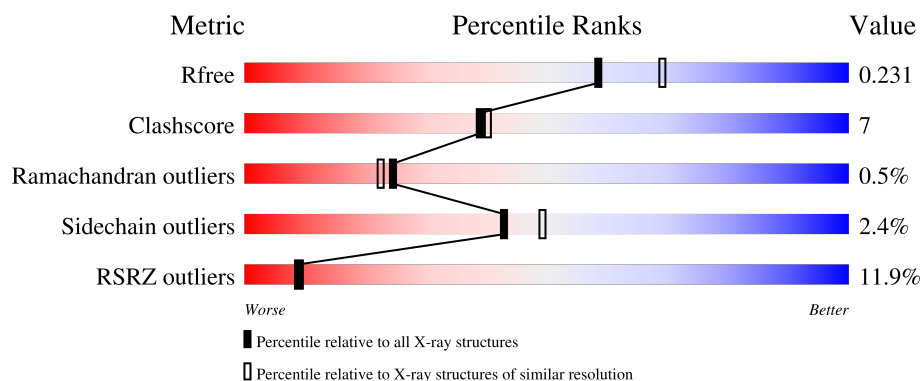
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	86% 12% ..
1	B	703	22% 80% 16% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11093 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.

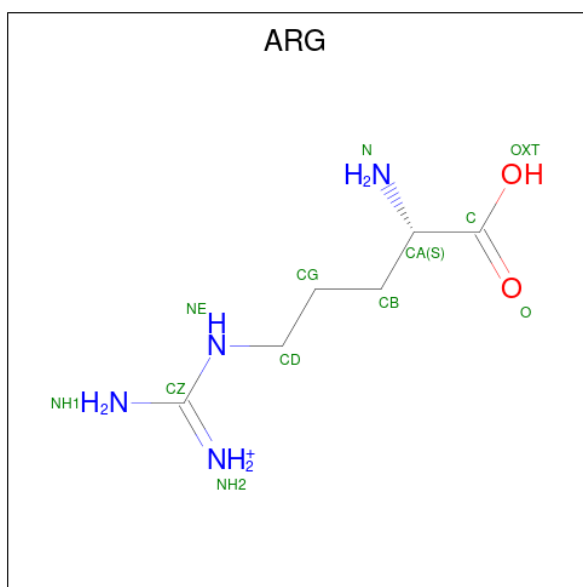
- Molecule 1 is a protein called Asp/Glu-specific dipeptidyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	1	0
			5511	3493	955	1038	25			
1	B	677	Total	C	N	O	S	0	0	0
			5038	3177	881	959	21			

There are 16 discrepancies between the modelled and reference sequences:

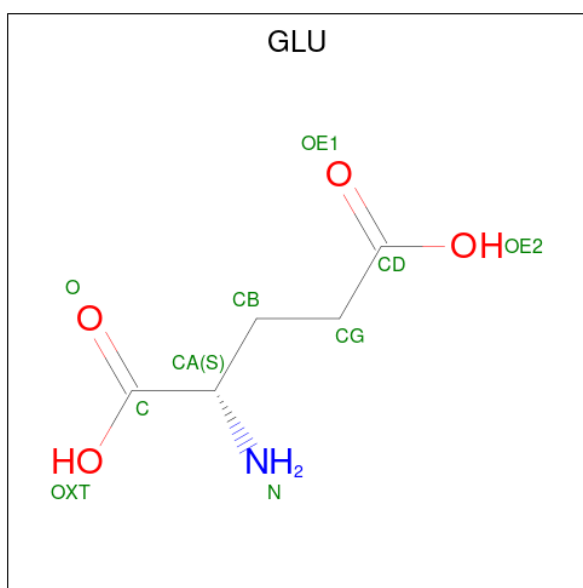
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP F8WQK8
A	652	ALA	SER	engineered mutation	UNP F8WQK8
A	718	HIS	-	expression tag	UNP F8WQK8
A	719	HIS	-	expression tag	UNP F8WQK8
A	720	HIS	-	expression tag	UNP F8WQK8
A	721	HIS	-	expression tag	UNP F8WQK8
A	722	HIS	-	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 ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	4	1		
2	B	1	Total	C	N	O	0	0
			11	6	4	1		

- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		
3	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	339	Total 339	O 339	0	0
5	B	161	Total 161	O 161	0	0

- 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	111.44Å 112.53Å 148.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.10 47.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.57-2.10) 98.8 (47.57-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.229 0.193 , 0.231	Depositor DCC
R_{free} test set	5385 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11093	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.53	0/5636	0.80	3/7623 (0.0%)
1	B	0.49	0/5144	0.85	7/6990 (0.1%)
All	All	0.51	0/10780	0.82	10/14613 (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	B	510	ASN	CA-C-N	7.85	129.65	119.84
1	B	510	ASN	C-N-CA	7.85	129.65	119.84
1	B	167	LYS	N-CA-C	-7.23	102.46	113.89
1	B	433	ILE	N-CA-C	-6.21	103.59	112.35
1	A	519	ASP	CA-C-N	6.03	125.74	119.05
1	A	519	ASP	C-N-CA	6.03	125.74	119.05
1	A	436	GLN	N-CA-C	5.84	118.39	111.33
1	B	171	ARG	CA-C-N	5.84	125.31	119.24
1	B	171	ARG	C-N-CA	5.84	125.31	119.24
1	B	453	GLN	N-CA-C	-5.78	105.89	113.12

There are no chirality outliers.

There are no planarity outliers.

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	5511	0	5354	67	0
1	B	5038	0	4631	73	0
2	A	11	0	12	0	0
2	B	11	0	12	0	0
3	A	10	0	6	2	0
3	B	10	0	6	1	0
4	B	2	0	0	0	0
5	A	339	0	0	6	0
5	B	161	0	0	5	0
All	All	11093	0	10021	140	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 (140) 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:313:MET:HE1	1:A:327:TYR:HB2	1.33	1.09
1:A:309:MET:HG2	1:A:313:MET:HE3	1.47	0.96
1:A:301:MET:HE3	1:A:395:TYR:HE1	1.40	0.84
1:A:298:ARG:HG3	1:A:302:ARG:HD3	1.59	0.84
1:B:182:TYR:OH	5:B:901:HOH:O	1.95	0.83
1:B:336:ARG:HH21	1:B:670:ARG:HH22	1.25	0.82
1:A:28:MET:HE3	1:A:51:TYR:HB2	1.60	0.81
1:B:168:ALA:O	1:B:170:SER:N	2.17	0.78
1:A:254:ARG:NH1	5:A:901:HOH:O	2.12	0.77
1:B:313:MET:SD	1:B:320:ASN:N	2.59	0.76
1:A:301:MET:HE3	1:A:395:TYR:CE1	2.22	0.74
1:A:44:GLN:HB2	1:A:660:ARG:HD3	1.70	0.74
1:A:411:ALA:H	1:A:436:GLN:NE2	1.90	0.69
1:A:22:ASP:OD1	1:A:37:ARG:NH2	2.26	0.69
1:A:359:GLU:HG2	1:A:560:MET:HE1	1.76	0.67
1:A:313:MET:HE2	1:A:323:TYR:CB	2.26	0.65
1:B:22:ASP:O	5:B:902:HOH:O	2.15	0.65
1:B:114:GLU:OE2	1:B:708:ARG:NH2	2.29	0.65
1:A:313:MET:HE2	1:A:323:TYR:HB3	1.79	0.64
1:B:449:VAL:HG22	1:B:450:GLU:H	1.63	0.63
1:A:474:SER:OG	1:A:488:TYR:OH	2.19	0.61
1:B:288:THR:OG1	1:B:350:ARG:NH1	2.34	0.61
1:A:350:ARG:NH2	5:A:906:HOH:O	2.33	0.61
1:B:392:ARG:HD2	1:B:535:LEU:HD21	1.82	0.60
1:B:313:MET:HG2	1:B:320:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ARG:NH1	1:B:531:GLU:OE2	2.36	0.59
1:B:359:GLU:HG2	1:B:560:MET:HE1	1.85	0.59
1:B:121:GLU:OE2	1:B:196:ARG:NH1	2.36	0.59
1:B:30:GLN:NE2	5:B:901:HOH:O	2.35	0.58
1:A:138:GLU:OE2	1:A:141:ARG:NH1	2.36	0.58
1:A:655:PRO:HB2	1:A:657:MET:HE3	1.86	0.57
1:B:298:ARG:O	1:B:302:ARG:HG3	2.04	0.57
1:A:433:ILE:HD13	1:A:516:LEU:HD11	1.85	0.57
1:B:96:SER:OG	1:B:98:GLN:O	2.17	0.56
1:B:293:ILE:HG21	1:B:390:ARG:HG2	1.88	0.56
1:B:348:SER:HB2	1:B:351:GLU:CG	2.36	0.56
1:A:28:MET:HE1	1:A:272:MET:HE3	1.86	0.55
1:A:341:ASN:HB3	1:A:345:ARG:HH12	1.71	0.55
1:A:123:GLU:OE2	1:A:175[B]:ARG:NH1	2.39	0.55
1:B:454:LEU:HA	1:B:457:ALA:HB3	1.88	0.55
1:B:63:VAL:HG13	1:B:122:VAL:HG13	1.89	0.55
1:A:256:VAL:HG21	1:A:657:MET:HE2	1.88	0.54
1:A:409:ALA:CB	1:A:521:MET:HE3	2.36	0.54
1:B:348:SER:HB2	1:B:351:GLU:HG2	1.90	0.54
1:A:652:ALA:HB2	3:A:802:GLU:C	2.33	0.54
1:B:299:ILE:HG13	1:B:300:GLU:N	2.23	0.54
1:A:271:ILE:HG12	1:A:656:VAL:HG22	1.90	0.54
1:A:39:LYS:NZ	1:A:46:GLU:OE2	2.41	0.54
1:B:320:ASN:O	1:B:324:ALA:N	2.41	0.54
1:B:346:ARG:O	1:B:347:ARG:NH1	2.42	0.53
1:B:389:LEU:HD21	1:B:538:GLU:HG2	1.90	0.53
1:B:652:ALA:HB2	3:B:804:GLU:C	2.34	0.53
1:A:445:TYR:CE1	1:A:450:GLU:HG3	2.44	0.53
1:B:568:PRO:HD3	5:B:901:HOH:O	2.08	0.52
1:A:498:TYR:HB2	1:A:521:MET:CE	2.39	0.52
1:B:413:ASP:O	1:B:415:ASP:N	2.43	0.52
1:A:410:PRO:CA	1:A:436:GLN:HE21	2.23	0.52
1:A:523:ARG:NH2	5:A:912:HOH:O	2.43	0.51
1:A:313:MET:CE	1:A:323:TYR:HB3	2.39	0.51
1:A:670:ARG:HB2	3:A:802:GLU:OE2	2.11	0.51
1:A:302:ARG:HD2	1:A:398:GLU:OE1	2.11	0.51
1:A:445:TYR:HE1	1:A:450:GLU:HG3	1.76	0.51
1:B:670:ARG:HH11	1:B:675:VAL:HA	1.75	0.50
1:B:63:VAL:HG22	1:B:124:ILE:HG12	1.93	0.50
1:A:149:GLU:HG2	5:A:1112:HOH:O	2.10	0.49
1:A:301:MET:HE1	1:A:461:ARG:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:OE1	1:B:351:GLU:N	2.44	0.49
1:B:331:GLN:HA	1:B:334:TYR:HB3	1.94	0.49
1:A:276:GLY:HA2	1:A:572:LEU:HD13	1.94	0.49
1:B:388:ASP:O	1:B:391:MET:HB2	2.13	0.49
1:A:213:SER:O	1:A:217:ASN:HB2	2.13	0.48
1:B:393:GLN:O	1:B:397:LEU:HB2	2.13	0.48
1:A:121:GLU:HG2	1:A:196:ARG:HG2	1.96	0.48
1:B:299:ILE:O	1:B:303:GLY:N	2.44	0.48
1:B:297:ILE:O	1:B:301:MET:HB2	2.14	0.48
1:A:410:PRO:HA	1:A:436:GLN:HE21	1.78	0.48
1:A:298:ARG:O	1:A:302:ARG:HB2	2.14	0.47
1:A:397:LEU:HD11	1:A:402:MET:HE3	1.96	0.47
1:B:90:GLN:HG2	1:B:120:LEU:HD22	1.97	0.47
1:B:347:ARG:HD3	1:B:347:ARG:HA	1.59	0.47
1:B:544:ALA:HB3	1:B:545:PRO:HD3	1.96	0.47
1:A:309:MET:CG	1:A:313:MET:HE3	2.32	0.47
1:B:291:SER:HA	1:B:295:ASN:HB2	1.95	0.47
1:A:411:ALA:N	1:A:436:GLN:NE2	2.62	0.47
1:A:293:ILE:HG21	1:A:390:ARG:HG2	1.96	0.47
1:B:272:MET:O	1:B:654:SER:HB3	2.15	0.47
1:A:514:ASP:O	1:A:515:ARG:HB3	2.14	0.46
1:B:168:ALA:HA	1:B:176:TYR:CE1	2.51	0.46
1:B:267:ASP:HB2	1:B:581:ILE:HD12	1.98	0.46
1:B:586:PRO:HG3	1:B:592:TYR:CZ	2.50	0.46
1:B:586:PRO:HG3	1:B:592:TYR:CE2	2.50	0.46
1:B:313:MET:HG2	1:B:320:ASN:HD22	1.80	0.46
1:A:313:MET:HE1	1:A:327:TYR:CB	2.23	0.45
1:B:271:ILE:HG12	1:B:656:VAL:HG22	1.99	0.45
1:A:63:VAL:HG13	1:A:122:VAL:HG13	1.97	0.45
1:A:498:TYR:HB2	1:A:521:MET:HE1	1.98	0.45
1:B:330:SER:OG	1:B:331:GLN:N	2.49	0.45
1:B:276:GLY:HA2	1:B:572:LEU:HD13	1.98	0.45
1:B:542:PHE:O	1:B:545:PRO:HD2	2.16	0.44
1:B:213:SER:O	1:B:217:ASN:HB2	2.17	0.44
1:B:670:ARG:NH1	1:B:675:VAL:HA	2.31	0.44
1:A:363:TRP:HB2	1:A:560:MET:HE3	2.00	0.44
1:B:28:MET:HE3	1:B:51:TYR:HB2	1.99	0.44
1:B:449:VAL:HG22	1:B:450:GLU:N	2.31	0.44
1:A:409:ALA:HB2	1:A:521:MET:HE3	1.98	0.44
1:A:301:MET:HE1	1:A:461:ARG:CG	2.47	0.44
1:A:544:ALA:HB3	1:A:545:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:MET:O	1:A:313:MET:HG3	2.19	0.43
1:B:695:TYR:O	1:B:699:ILE:HG12	2.18	0.43
1:A:469:GLU:H	1:A:469:GLU:CD	2.26	0.43
1:B:389:LEU:CD2	1:B:538:GLU:HG2	2.49	0.43
1:B:168:ALA:C	1:B:170:SER:N	2.76	0.43
1:A:512:ASP:O	1:A:516:LEU:HB2	2.19	0.43
1:A:450:GLU:HG2	5:A:987:HOH:O	2.19	0.43
1:B:295:ASN:O	1:B:299:ILE:HG23	2.19	0.43
1:B:473:ILE:HG13	1:B:527:SER:HB2	2.01	0.43
1:B:336:ARG:HH22	1:B:649:GLY:H	1.67	0.42
1:B:563:GLN:HB3	1:B:564:PRO:HD3	2.01	0.42
1:A:174:TYR:CE2	1:A:193:LYS:HG2	2.54	0.42
1:B:22:ASP:OD2	1:B:37:ARG:NE	2.51	0.42
1:B:587:ARG:NH2	5:B:914:HOH:O	2.52	0.42
1:A:468:ALA:O	1:A:476:ARG:HD3	2.19	0.42
1:A:168:ALA:O	1:A:176:TYR:OH	2.32	0.41
1:B:231:ARG:HD2	1:B:233:TYR:CE1	2.55	0.41
1:B:449:VAL:CG2	1:B:450:GLU:H	2.31	0.41
1:B:542:PHE:C	1:B:545:PRO:HD2	2.46	0.41
1:A:394:ARG:HD3	5:A:923:HOH:O	2.20	0.41
1:B:210:LYS:HB2	1:B:213:SER:HB3	2.01	0.41
1:A:239:ASN:HA	1:A:240:PRO:HD2	1.92	0.41
1:B:39:LYS:HE2	1:B:45:LEU:O	2.21	0.41
1:B:159:LEU:O	1:B:163:ILE:HG12	2.21	0.41
1:A:363:TRP:CD1	1:A:560:MET:HG3	2.56	0.41
1:B:354:LEU:O	1:B:357:GLN:HG2	2.21	0.41
1:A:294:ASP:HA	1:A:394:ARG:HD2	2.02	0.41
1:A:507:PHE:CD2	1:A:508:MET:HE3	2.55	0.41
1:B:218:TRP:CD1	1:B:335:LYS:HB3	2.56	0.41
1:A:482:TYR:CZ	1:A:491:MET:HG3	2.56	0.40
1:A:167:LYS:O	1:A:168:ALA:HB3	2.21	0.40
1:B:432:SER:HA	1:B:435:LYS:H	1.86	0.40
1:B:357:GLN:HA	1:B:360:VAL:HG12	2.03	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	696/703 (99%)	675 (97%)	20 (3%)	1 (0%)	48	50
1	B	669/703 (95%)	633 (95%)	30 (4%)	6 (1%)	14	10
All	All	1365/1406 (97%)	1308 (96%)	50 (4%)	7 (0%)	24	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	VAL
1	B	414	SER
1	B	589	VAL
1	B	146	SER
1	B	169	ALA
1	B	450	GLU
1	B	511	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	563/583 (97%)	549 (98%)	14 (2%)	42	48
1	B	470/583 (81%)	459 (98%)	11 (2%)	44	51
All	All	1033/1166 (89%)	1008 (98%)	25 (2%)	43	49

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	138	GLU
1	A	140	GLU
1	A	149	GLU
1	A	162	GLU
1	A	193	LYS
1	A	236	LYS
1	A	302	ARG
1	A	389	LEU
1	A	414	SER
1	A	449	VAL
1	A	515	ARG
1	A	572	LEU
1	A	599	GLU
1	B	63	VAL
1	B	330	SER
1	B	344	ILE
1	B	351	GLU
1	B	433	ILE
1	B	462	TYR
1	B	470	LYS
1	B	473	ILE
1	B	492	ILE
1	B	503	ARG
1	B	629	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	GLN
1	A	532	HIS
1	A	632	ASN
1	B	261	GLN
1	B	320	ASN
1	B	565	ASN

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ARG	A	801	-	9,10,11	0.56	0	5,11,13	0.26	0
3	GLU	A	802	-	8,9,9	1.25	1 (12%)	8,11,11	1.23	1 (12%)
3	GLU	B	804	-	8,9,9	1.12	1 (12%)	8,11,11	1.14	1 (12%)
2	ARG	B	803	-	9,10,11	0.45	0	5,11,13	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	A	801	-	-	0/8/9/11	-
3	GLU	A	802	-	-	1/9/9/9	-
3	GLU	B	804	-	-	2/9/9/9	-
2	ARG	B	803	-	-	0/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	GLU	OXT-C	-2.05	1.24	1.30
3	B	804	GLU	OXT-C	-2.03	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	GLU	OXT-C-O	-2.74	117.85	124.08
3	B	804	GLU	OXT-C-O	-2.43	118.58	124.08

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	804	GLU	OXT-C-CA-CB
3	B	804	GLU	O-C-CA-CB
3	A	802	GLU	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GLU	2	0
3	B	804	GLU	1	0

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	697/703 (99%)	-0.14	6 (0%) 81 83	25, 41, 64, 84	1 (0%)
1	B	677/703 (96%)	0.92	157 (23%) 2 2	28, 58, 157, 192	0
All	All	1374/1406 (97%)	0.38	163 (11%) 9 9	25, 47, 146, 192	1 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	TYR	7.1
1	B	407	SER	5.4
1	B	409	ALA	5.4
1	B	169	ALA	5.4
1	B	326	LYS	5.2
1	B	439	ALA	5.1
1	B	325	ALA	5.0
1	B	310	LEU	5.0
1	B	322	MET	4.8
1	B	430	LEU	4.7
1	B	147	GLY	4.7
1	B	489	VAL	4.7
1	A	342	TRP	4.6
1	B	485	ALA	4.6
1	B	404	ILE	4.5
1	B	308	VAL	4.5
1	B	315	ALA	4.5
1	B	473	ILE	4.4
1	B	309	MET	4.4
1	B	441	PHE	4.3
1	B	433	ILE	4.3
1	B	408	ASN	4.2
1	B	321	ILE	4.2
1	B	447	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	411	ALA	4.2
1	B	449	VAL	4.2
1	B	457	ALA	4.1
1	B	453	GLN	4.1
1	B	170	SER	4.1
1	B	405	GLU	4.0
1	B	479	ILE	4.0
1	B	306	GLN	4.0
1	B	402	MET	4.0
1	B	414	SER	4.0
1	B	394	ARG	4.0
1	B	143	LYS	3.9
1	B	403	GLY	3.9
1	B	316	ASP	3.8
1	A	168	ALA	3.8
1	B	466	ILE	3.8
1	B	498	TYR	3.7
1	B	460	THR	3.7
1	B	313	MET	3.7
1	B	401	LEU	3.7
1	B	524	PHE	3.7
1	B	468	ALA	3.7
1	B	526	ALA	3.7
1	B	445	TYR	3.7
1	B	459	LEU	3.6
1	B	406	MET	3.6
1	B	142	ILE	3.6
1	B	444	ASP	3.6
1	B	504	PHE	3.6
1	B	463	ALA	3.6
1	B	454	LEU	3.6
1	B	327	TYR	3.6
1	B	166	LYS	3.5
1	B	400	ILE	3.5
1	B	314	LEU	3.5
1	B	300	GLU	3.5
1	B	522	SER	3.5
1	B	525	ALA	3.4
1	B	442	ASN	3.4
1	B	520	PRO	3.4
1	B	304	ILE	3.4
1	B	329	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	536	ALA	3.4
1	B	396	LEU	3.4
1	B	434	ARG	3.3
1	B	438	GLU	3.3
1	B	511	PRO	3.2
1	B	148	LEU	3.2
1	B	415	ASP	3.2
1	B	500	SER	3.2
1	B	509	LYS	3.2
1	B	397	LEU	3.1
1	B	465	ARG	3.1
1	B	443	LYS	3.1
1	B	448	GLU	3.1
1	B	523	ARG	3.1
1	B	168	ALA	3.0
1	B	320	ASN	3.0
1	B	324	ALA	3.0
1	B	514	ASP	3.0
1	B	507	PHE	3.0
1	B	290	TRP	2.9
1	B	305	LEU	2.9
1	B	435	LYS	2.9
1	B	317	PRO	2.9
1	B	462	TYR	2.9
1	B	146	SER	2.9
1	B	458	LEU	2.9
1	B	307	ASP	2.9
1	B	299	ILE	2.9
1	B	482	TYR	2.9
1	B	491	MET	2.8
1	B	432	SER	2.8
1	B	530	TYR	2.8
1	B	141	ARG	2.8
1	B	487	ALA	2.8
1	B	450	GLU	2.7
1	B	528	VAL	2.6
1	B	508	MET	2.6
1	B	344	ILE	2.6
1	B	328	ALA	2.6
1	B	493	PHE	2.6
1	B	389	LEU	2.6
1	A	483	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	455	ALA	2.5
1	B	516	LEU	2.5
1	B	393	GLN	2.5
1	B	446	SER	2.5
1	B	302	ARG	2.4
1	B	312	GLU	2.4
1	B	398	GLU	2.4
1	B	410	PRO	2.4
1	B	412	ALA	2.4
1	B	293	ILE	2.4
1	B	451	LYS	2.4
1	B	477	GLU	2.4
1	B	431	GLN	2.4
1	B	336	ARG	2.4
1	B	539	VAL	2.4
1	B	303	GLY	2.3
1	A	93	LYS	2.3
1	B	413	ASP	2.3
1	B	562	GLY	2.3
1	B	534	LYS	2.3
1	B	155	TYR	2.3
1	B	610	TRP	2.3
1	A	717	PHE	2.2
1	B	518	ARG	2.2
1	B	395	TYR	2.2
1	A	345	ARG	2.2
1	B	399	GLY	2.2
1	B	502	GLU	2.2
1	B	503	ARG	2.2
1	B	153	PRO	2.2
1	B	297	ILE	2.2
1	B	535	LEU	2.2
1	B	521	MET	2.2
1	B	452	ASP	2.2
1	B	499	ALA	2.1
1	B	139	LEU	2.1
1	B	513	ARG	2.1
1	B	98	GLN	2.1
1	B	340	ALA	2.1
1	B	140	GLU	2.1
1	B	149	GLU	2.1
1	B	22	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	472	PRO	2.1
1	B	440	PHE	2.1
1	B	542	PHE	2.1
1	B	89	ASP	2.1
1	B	331	GLN	2.1
1	B	492	ILE	2.1
1	B	330	SER	2.1
1	B	464	GLU	2.0
1	B	456	ILE	2.0
1	B	437	PHE	2.0
1	B	510	ASN	2.0
1	B	145	PRO	2.0
1	B	467	PRO	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](#)

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	ARG	B	803	11/12	0.92	0.11	48,50,53,56	0
3	GLU	B	804	10/10	0.92	0.10	48,49,51,52	0
3	GLU	A	802	10/10	0.96	0.07	27,35,39,39	0
4	CL	B	801	1/1	0.96	0.07	56,56,56,56	0
2	ARG	A	801	11/12	0.97	0.06	26,31,38,40	0
4	CL	B	802	1/1	0.97	0.15	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.