Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2020 – 09:21 PM BST

PDB ID	:	5JWI
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.; Djinovic-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 (i) symbol.

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

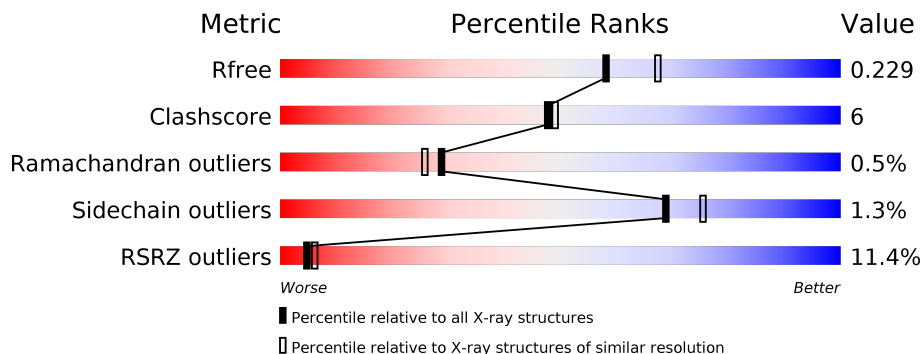|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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	Percentile Ranks	Value
Rfree		0.229
Clashscore		6
Ramachandran outliers		0.5%
Sidechain outliers		1.3%
RSRZ outliers		11.4%

Worse ← → *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	703	88% 11% •
1	B	703	22% (upper bar) / 81% 15% • •

2 Entry composition (i)

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 5511	C 3493	N 955	O 1038	S 25	0	1	0
1	B	677	Total 5038	C 3177	N 881	O 959	S 21	0	0	0

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 (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).
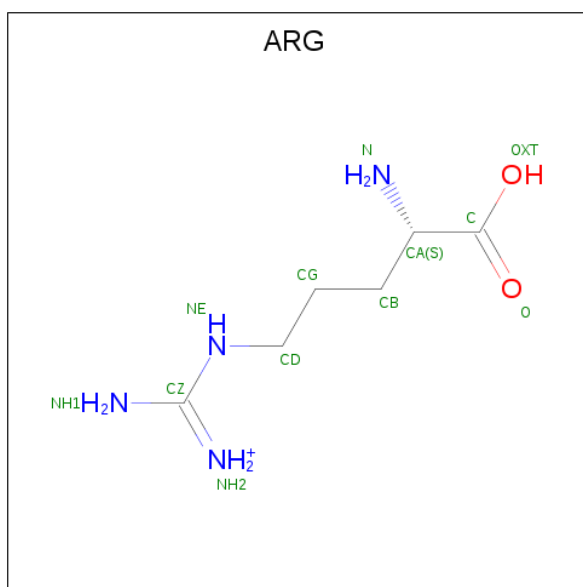
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 11	C 6	N 4	O 1	0	0
2	B	1	Total 11	C 6	N 4	O 1	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).
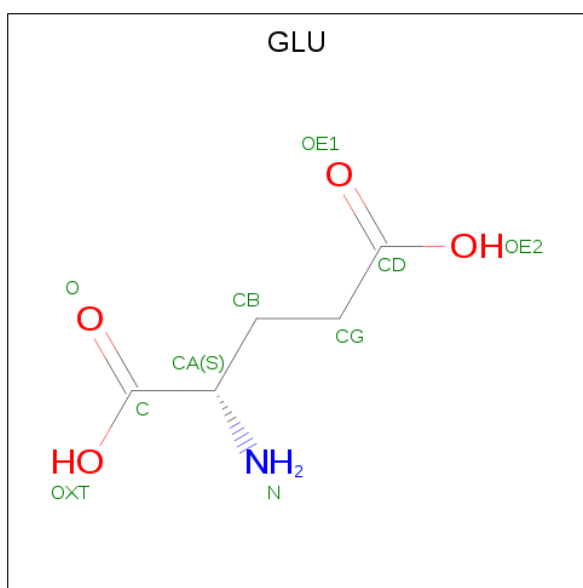
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 5	N 1	O 4	0	0
3	B	1	Total 10	C 5	N 1	O 4	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: 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

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
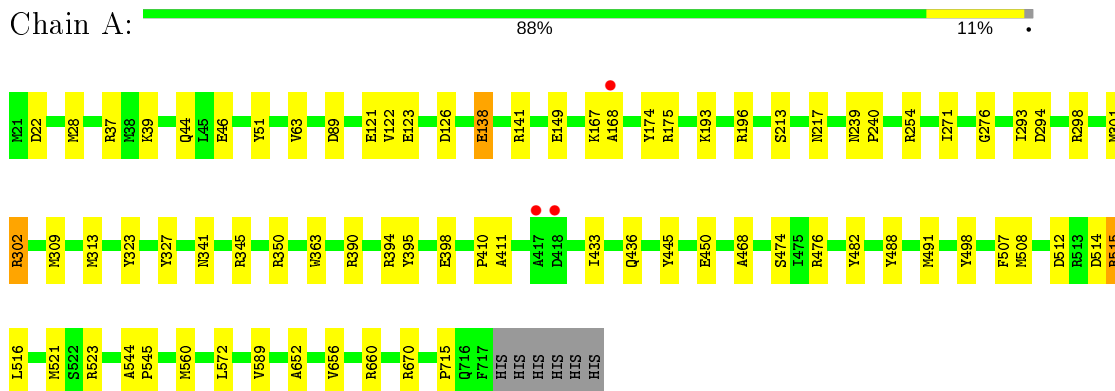
- Molecule 1: Asp/Glu-specific dipeptidyl-peptidase
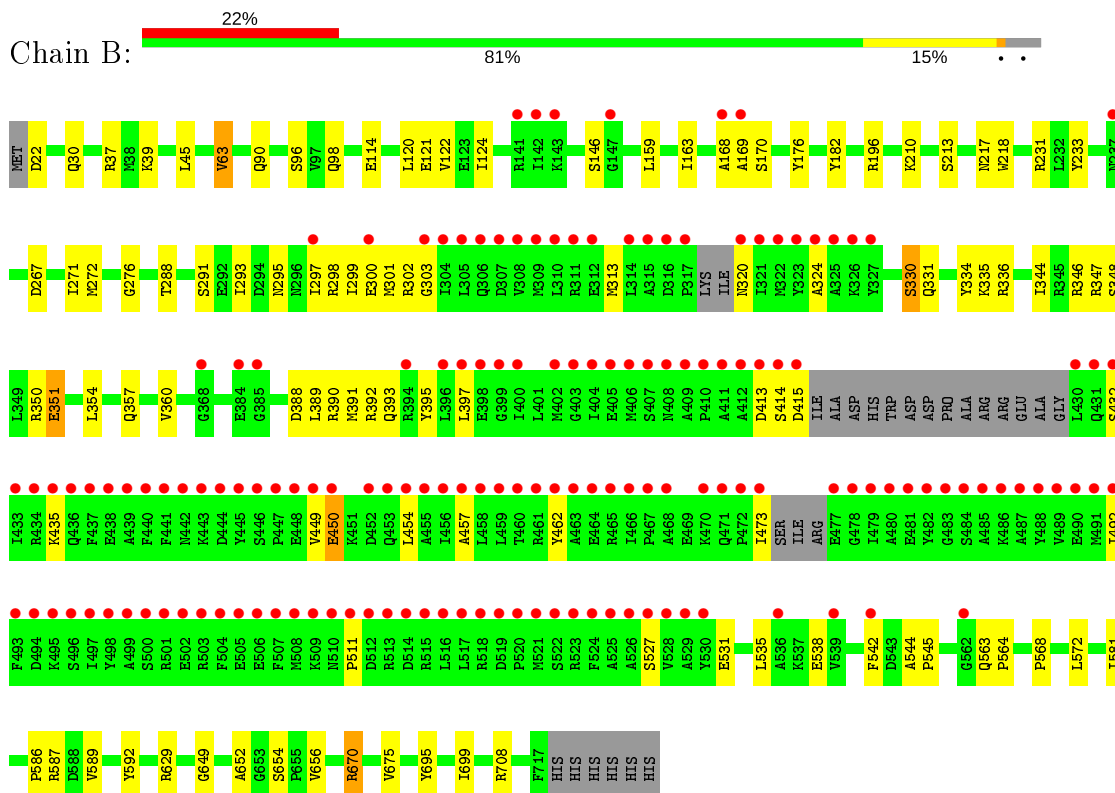
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.229 0.191 , 0.229	Depositor DCC
R_{free} test set	5385 reflections (4.99%)	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)	0.30 , 50.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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[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 (i)

5.1 Standard geometry (i)

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	0.43	0/5636	0.55	2/7623 (0.0%)
1	B	0.38	0/5144	0.54	1/6990 (0.0%)
All	All	0.41	0/10780	0.55	3/14613 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	302	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	670	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	302	ARG	NE-CZ-NH1	5.09	122.85	120.30

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	5511	0	5354	57	0
1	B	5038	0	4631	69	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	126	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 (126) 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: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: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:44:GLN:HB2	1:A:660:ARG:HD3	1.70	0.74
1:A:498:TYR:HB2	1:A:521:MET:HE1	1.70	0.72
1:A:313:MET:HE3	1:A:327:TYR:HB2	1.72	0.70
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: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:CE	1:A:327:TYR:HB2	2.26	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
1:B:392:ARG:NH1	1:B:531:GLU:OE2	2.36	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: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:341:ASN:HB3	1:A:345:ARG:HH12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:348:SER:HB2	1:B:351:GLU:HG2	1.90	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: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:313:MET:HE1	1:A:323:TYR:O	2.10	0.52
1:B:413:ASP:O	1:B:415:ASP:N	2.43	0.52
1:A:313:MET:CE	1:A:323:TYR:HB3	2.39	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: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:498:TYR:HB2	1:A:521:MET:CE	2.39	0.49
1:A:652:ALA:HB2	3:A:802:GLU:C	2.33	0.49
1:B:351:GLU:N	1:B:351:GLU:OE1	2.44	0.49
1:A:309:MET:HG2	1:A:313:MET:CE	2.41	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:A:313:MET:HE2	1:A:323:TYR:HB3	1.95	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:A:301:MET:HE3	1:A:395:TYR:HE1	1.78	0.48
1:B:299:ILE:O	1:B:303:GLY:N	2.44	0.48
1:B:652:ALA:HB2	3:B:804:GLU:C	2.34	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:B:90:GLN:HG2	1:B:120:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:309:MET:HG2	1:A:313:MET:HE3	1.96	0.46
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: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: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:B:449:VAL:HG22	1:B:450:GLU:N	2.31	0.44
1:A:544:ALA:HB3	1:A:545:PRO:HD3	1.99	0.43
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:B:389:LEU:CD2	1:B:538:GLU:HG2	2.49	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:A:301:MET:CE	1:A:395:TYR:HE1	2.32	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:28:MET:CE	1:A:51:TYR:HB2	2.50	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:A:394:ARG:HD3	5:A:923:HOH:O	2.20	0.41
1:A:313:MET:HE2	1:A:323:TYR:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:507:PHE:CD2	1:A:508:MET:HE2	2.56	0.41
1:B:159:LEU:O	1:B:163:ILE:HG12	2.21	0.41
1:B:39:LYS:HE2	1:B:45:LEU:O	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:309:MET:SD	1:A:313:MET:HE3	2.60	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%)	51	54
1	B	669/703 (95%)	633 (95%)	30 (4%)	6 (1%)	17	12
All	All	1365/1406 (97%)	1308 (96%)	50 (4%)	7 (0%)	29	26

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

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Mol	Chain	Res	Type
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%)	558 (99%)	5 (1%)	78	84
1	B	470/583 (81%)	462 (98%)	8 (2%)	60	67
All	All	1033/1166 (89%)	1020 (99%)	13 (1%)	69	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASP
1	A	126	ASP
1	A	138	GLU
1	A	515	ARG
1	A	715	PRO
1	B	63	VAL
1	B	330	SER
1	B	344	ILE
1	B	351	GLU
1	B	395	TYR
1	B	462	TYR
1	B	492	ILE
1	B	629	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	GLN
1	B	217	ASN

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Mol	Chain	Res	Type
1	B	320	ASN
1	B	332	ASN
1	B	565	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 monosaccharides 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	B	803	-	9,10,11	0.46	0	5,11,13	0.43	0
2	ARG	A	801	-	9,10,11	0.55	0	5,11,13	0.27	0
3	GLU	A	802	-	2,9,9	0.88	0	2,11,11	0.66	0
3	GLU	B	804	-	2,9,9	0.54	0	2,11,11	0.62	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.

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

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.

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 (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	697/703 (99%)	-0.16	3 (0%)	92	93	26, 41, 64, 84	0
1	B	677/703 (96%)	1.23	154 (22%)	0	0	28, 58, 157, 192	0
All	All	1374/1406 (97%)	0.52	157 (11%)	5	6	26, 47, 146, 192	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	TYR	10.9
1	B	517	LEU	10.9
1	B	169	ALA	10.4
1	B	439	ALA	10.3
1	B	489	VAL	10.1
1	B	406	MET	9.8
1	B	403	GLY	9.8
1	B	435	LYS	9.8
1	B	408	ASN	9.8
1	B	432	SER	9.5
1	B	498	TYR	9.4
1	B	483	GLY	8.9
1	B	409	ALA	8.7
1	B	525	ALA	8.3
1	B	487	ALA	8.3
1	B	482	TYR	8.2
1	B	493	PHE	8.1
1	B	466	ILE	8.1
1	B	448	GLU	8.0
1	B	458	LEU	7.9
1	B	497	ILE	7.8
1	B	459	LEU	7.7
1	B	404	ILE	7.6
1	B	463	ALA	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	447	PRO	7.6
1	B	440	PHE	7.5
1	B	433	ILE	7.5
1	B	442	ASN	7.3
1	B	304	ILE	7.3
1	B	452	ASP	7.2
1	B	322	MET	7.1
1	B	528	VAL	7.1
1	B	434	ARG	7.0
1	B	488	TYR	6.9
1	B	511	PRO	6.9
1	B	436	GLN	6.9
1	B	522	SER	6.8
1	B	308	VAL	6.7
1	B	485	ALA	6.6
1	B	504	PHE	6.6
1	B	407	SER	6.6
1	B	445	TYR	6.6
1	B	438	GLU	6.5
1	B	453	GLN	6.5
1	B	490	GLU	6.5
1	B	478	GLY	6.4
1	B	397	LEU	6.4
1	B	510	ASN	6.3
1	B	521	MET	6.3
1	B	454	LEU	6.2
1	B	415	ASP	6.0
1	B	437	PHE	6.0
1	B	516	LEU	6.0
1	B	506	GLU	5.9
1	B	468	ALA	5.9
1	B	481	GLU	5.9
1	B	507	PHE	5.8
1	B	494	ASP	5.8
1	B	399	GLY	5.8
1	B	479	ILE	5.7
1	B	519	ASP	5.7
1	B	501	ARG	5.7
1	B	514	ASP	5.6
1	B	523	ARG	5.5
1	B	508	MET	5.5
1	B	496	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	509	LYS	5.4
1	B	492	ILE	5.4
1	B	315	ALA	5.4
1	B	512	ASP	5.4
1	B	524	PHE	5.3
1	B	460	THR	5.2
1	B	405	GLU	5.2
1	B	306	GLN	5.1
1	B	513	ARG	5.1
1	B	310	LEU	5.0
1	B	529	ALA	5.0
1	B	414	SER	5.0
1	B	491	MET	4.9
1	B	530	TYR	4.9
1	B	410	PRO	4.9
1	B	480	ALA	4.8
1	B	413	ASP	4.8
1	B	473	ILE	4.7
1	B	431	GLN	4.6
1	B	321	ILE	4.5
1	B	402	MET	4.5
1	B	515	ARG	4.5
1	B	143	LYS	4.5
1	B	307	ASP	4.5
1	B	505	GLU	4.4
1	B	320	ASN	4.4
1	B	464	GLU	4.4
1	B	500	SER	4.4
1	B	520	PRO	4.4
1	B	309	MET	4.3
1	B	484	SER	4.3
1	B	305	LEU	4.3
1	B	444	ASP	4.3
1	B	326	LYS	4.2
1	B	325	ALA	4.1
1	B	461	ARG	4.1
1	B	527	SER	4.1
1	B	542	PHE	4.1
1	B	311	ARG	4.1
1	B	526	ALA	4.1
1	B	141	ARG	4.0
1	B	450	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	462	TYR	3.9
1	B	412	ALA	3.9
1	B	536	ALA	3.8
1	B	300	GLU	3.8
1	B	495	LYS	3.7
1	B	411	ALA	3.6
1	B	327	TYR	3.6
1	B	486	LYS	3.6
1	B	457	ALA	3.5
1	B	499	ALA	3.5
1	B	455	ALA	3.5
1	B	465	ARG	3.4
1	B	477	GLU	3.4
1	B	502	GLU	3.3
1	B	446	SER	3.2
1	B	316	ASP	3.2
1	B	443	LYS	3.2
1	A	168	ALA	3.1
1	B	562	GLY	3.0
1	B	503	ARG	3.0
1	B	324	ALA	3.0
1	B	449	VAL	2.9
1	B	518	ARG	2.9
1	B	368	GLY	2.9
1	B	539	VAL	2.8
1	B	472	PRO	2.8
1	B	317	PRO	2.7
1	B	314	LEU	2.7
1	B	441	PHE	2.7
1	B	400	ILE	2.6
1	B	303	GLY	2.6
1	B	297	ILE	2.5
1	B	394	ARG	2.5
1	B	385	GLY	2.5
1	B	168	ALA	2.4
1	A	418	ASP	2.4
1	B	430	LEU	2.3
1	B	470	LYS	2.3
1	B	312	GLU	2.3
1	A	417	ALA	2.2
1	B	147	GLY	2.2
1	B	237	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	396	LEU	2.2
1	B	471	GLN	2.1
1	B	398	GLU	2.1
1	B	142	ILE	2.1
1	B	384	GLU	2.1
1	B	467	PRO	2.0
1	B	456	ILE	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, 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(Å^2)	Q<0.9
2	ARG	B	803	11/12	0.85	0.17	48,50,53,56	0
3	GLU	B	804	10/10	0.91	0.14	48,49,51,52	0
3	GLU	A	802	10/10	0.94	0.16	27,35,39,39	0
2	ARG	A	801	11/12	0.96	0.15	26,31,38,40	0
4	CL	B	801	1/1	0.98	0.12	56,56,56,56	0
4	CL	B	802	1/1	0.99	0.07	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.