Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 09:18 PM BST

PDB ID	:	5JWG
Title	:	Crystal structure of Porphyromonas endodontalis DPP11 in complex with dipeptide Arg-Asp
Authors	:	Bezerra, G.A.; Fedosyuk, S.; Ohara-Nemoto, Y.; Nemoto, T.K.; Djinovic-Carugo, K.
Deposited on	:	2016-05-12
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

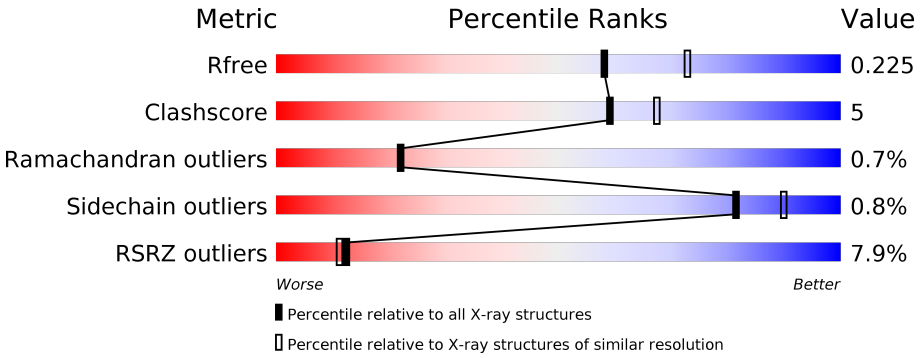
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	2% 89% 10%
1	B	703	13% 88% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11235 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.

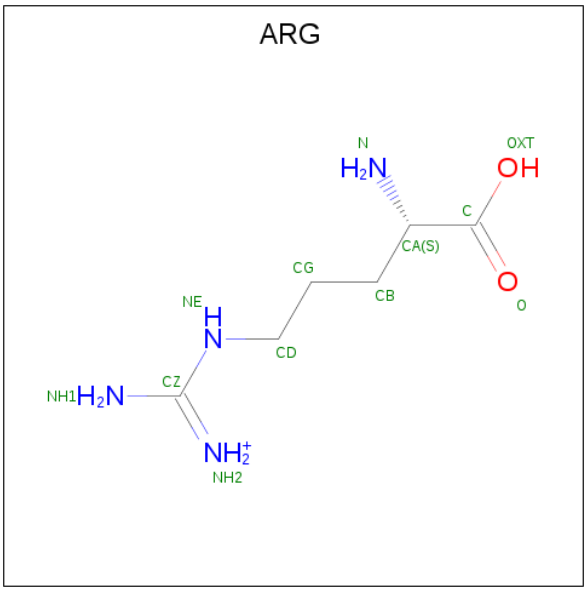
- Molecule 1 is a protein called Asp/Glu-specific dipeptidyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	1	0
			5558	3517	967	1048	26			
1	B	695	Total	C	N	O	S	0	0	0
			5211	3313	896	979	23			

There are 16 discrepancies between the modelled and reference sequences:

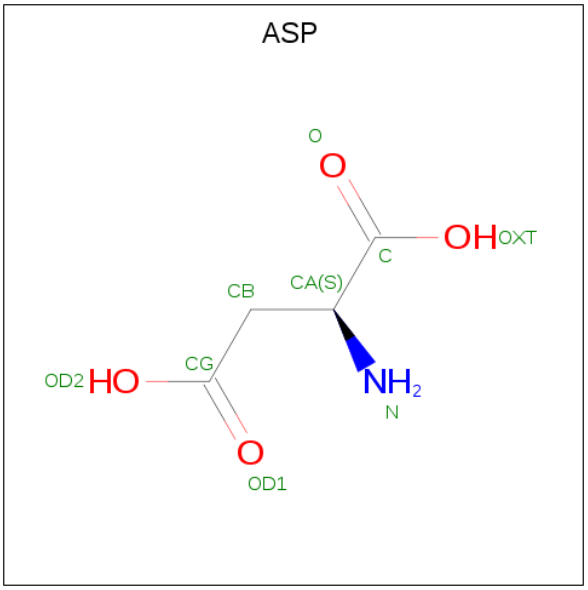
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP F8WQK8
A	652	ALA	SER	engineered mutation	UNP F8WQK8
A	718	HIS	-	expression tag	UNP F8WQK8
A	719	HIS	-	expression tag	UNP F8WQK8
A	720	HIS	-	expression tag	UNP F8WQK8
A	721	HIS	-	expression tag	UNP F8WQK8
A	722	HIS	-	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: $C_6H_{15}N_4O_2$).



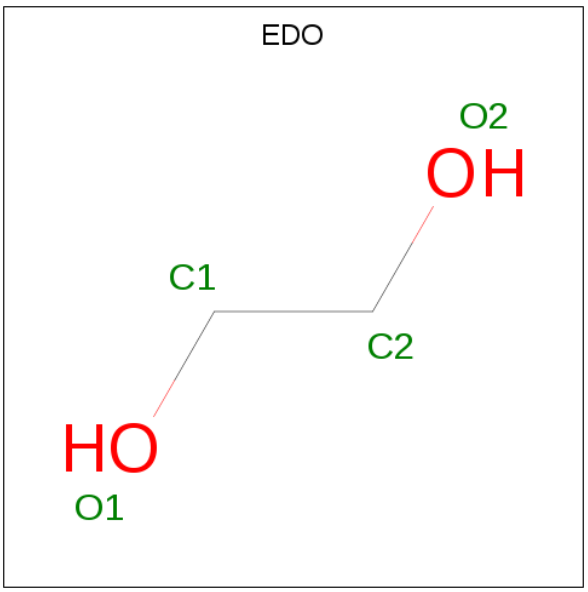
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 11 6 4 1	0	0
2	B	1	Total C N O 11 6 4 1	0	0

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 4 1 4	0	0
3	B	1	Total C N O 9 4 1 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

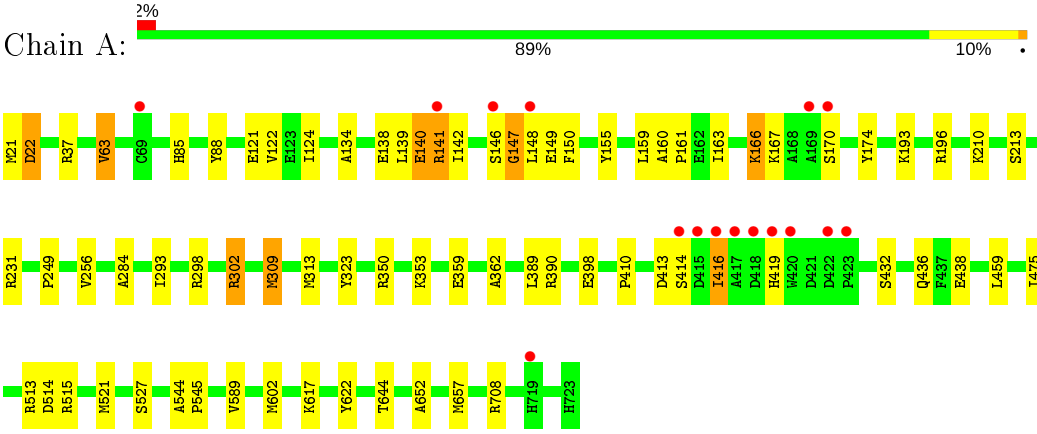
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	283	Total O 283 283	0	0
6	B	138	Total O 138 138	0	0

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.

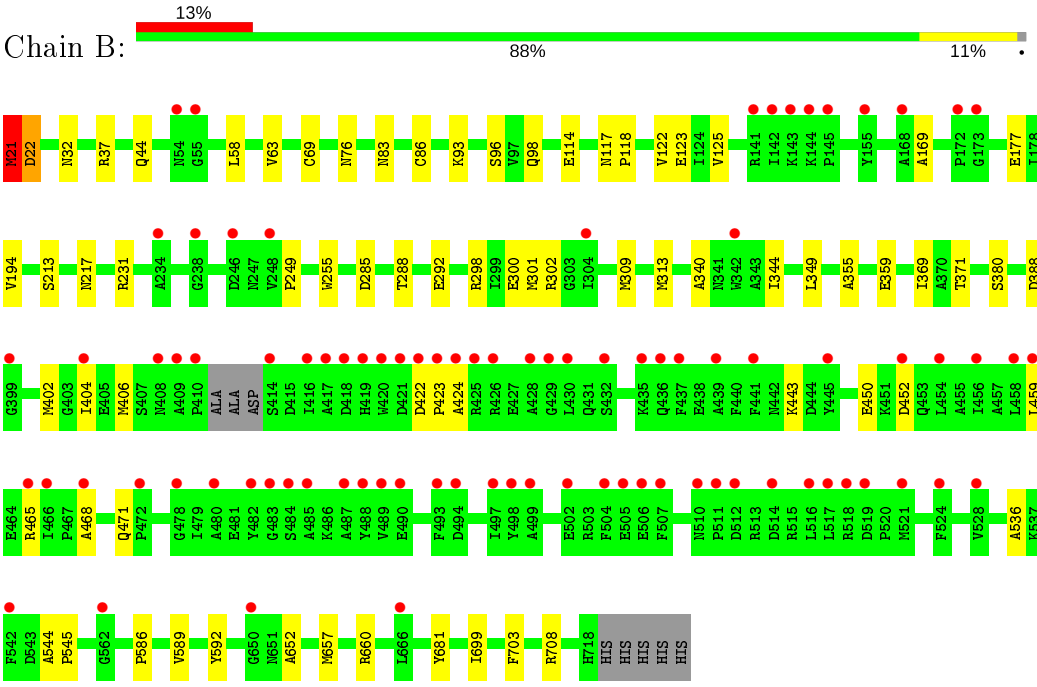
- Molecule 1: Asp/Glu-specific dipeptidyl-peptidase

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.81Å 114.40Å 147.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 2.20 45.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.24-2.20) 99.5 (45.24-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.227 0.184 , 0.225	Depositor DCC
R_{free} test set	4811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11235	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: NA, EDO

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	0/5687	0.58	3/7693 (0.0%)
1	B	0.40	0/5325	0.56	3/7232 (0.0%)
All	All	0.42	0/11012	0.57	6/14925 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	MET	CB-CG-SD	-9.55	83.74	112.40
1	A	302	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	302	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	22	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	708	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	B	21	MET	CG-SD-CE	-5.04	92.14	100.20

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	5558	0	5374	54	0
1	B	5211	0	4841	44	0
2	A	11	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	11	0	12	0	0
3	A	9	0	4	1	0
3	B	9	0	4	1	0
4	A	4	0	6	2	0
5	A	1	0	0	0	0
6	A	283	0	0	4	0
6	B	138	0	0	3	0
All	All	11235	0	10253	98	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 5.

All (98) 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:SD	6:A:1133:HOH:O	2.29	0.91
1:A:657:MET:SD	6:A:1158:HOH:O	2.30	0.89
1:A:416:ILE:HA	1:A:513:ARG:HE	1.39	0.86
1:B:388:ASP:HA	1:B:391:MET:HB3	1.56	0.85
1:A:147:GLY:O	1:A:148:LEU:HG	1.85	0.76
1:A:298:ARG:HG3	1:A:302:ARG:HD3	1.68	0.74
1:A:22:ASP:HB2	1:A:37:ARG:NH2	2.05	0.72
1:B:300:GLU:HG3	1:B:301:MET:HE2	1.73	0.70
1:A:514:ASP:O	1:A:515:ARG:HB3	1.97	0.65
1:B:22:ASP:O	6:B:901:HOH:O	2.15	0.65
1:A:309:MET:HB3	1:A:313:MET:HE3	1.81	0.63
1:B:298:ARG:HG3	1:B:302:ARG:HD3	1.79	0.63
1:A:498:TYR:HB2	1:A:521:MET:HE1	1.83	0.60
1:A:617:LYS:NZ	6:A:904:HOH:O	2.34	0.59
1:B:213:SER:O	1:B:217:ASN:HB2	2.01	0.59
1:A:166:LYS:O	1:A:170:SER:HB3	2.02	0.59
1:B:96:SER:OG	1:B:98:GLN:O	2.14	0.59
1:B:389:LEU:HD11	1:B:538:GLU:HB3	1.84	0.58
1:A:138:GLU:HG2	1:A:159:LEU:HD22	1.84	0.58
1:A:231:ARG:HD3	1:A:249:PRO:HB3	1.86	0.58
1:B:340:ALA:O	1:B:344:ILE:HG12	2.04	0.58
1:A:148:LEU:HD12	1:A:544:ALA:O	2.04	0.58
1:A:146:SER:O	1:A:147:GLY:C	2.43	0.57
1:A:166:LYS:HG2	1:A:167:LYS:N	2.19	0.57
1:B:114:GLU:OE2	1:B:708:ARG:NH2	2.37	0.56
1:B:22:ASP:OD2	1:B:37:ARG:NE	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD22	1:A:150:PHE:CE1	2.41	0.56
1:B:344:ILE:HD13	1:B:349:LEU:HD12	1.87	0.55
1:A:134:ALA:HB1	1:A:163:ILE:HD12	1.89	0.54
1:B:123:GLU:HG2	1:B:194:VAL:HG22	1.90	0.54
1:A:146:SER:HB3	1:A:149:GLU:OE1	2.07	0.53
1:A:544:ALA:HB3	1:A:545:PRO:HD3	1.89	0.53
1:A:139:LEU:C	1:A:140:GLU:O	2.45	0.53
1:A:213:SER:O	1:A:217:ASN:HB2	2.07	0.53
1:A:210:LYS:HE2	1:A:213:SER:HB2	1.92	0.52
1:A:432:SER:O	1:A:436:GLN:HG2	2.09	0.52
1:A:21:MET:N	1:A:644:THR:HG1	2.08	0.51
1:A:142:ILE:HD11	1:A:155:TYR:OH	2.10	0.51
1:A:438:GLU:OE2	1:A:501:ARG:NH2	2.44	0.51
1:B:355:ALA:O	1:B:359:GLU:HG2	2.11	0.50
1:A:359:GLU:HA	4:A:803:EDO:H11	1.93	0.50
1:A:459:LEU:HD11	1:A:475:ILE:HD13	1.94	0.49
1:B:285:ASP:OD2	1:B:380:SER:OG	2.24	0.49
1:B:21:MET:HA	1:B:681:TYR:OH	2.12	0.49
1:A:652:ALA:HB2	3:A:802:ASP:C	2.33	0.49
1:B:288:THR:O	1:B:292:GLU:HG3	2.13	0.49
1:A:148:LEU:HD22	1:A:150:PHE:CD1	2.49	0.48
1:A:63:VAL:HG22	1:A:124:ILE:HG12	1.96	0.48
1:A:63:VAL:HG13	1:A:122:VAL:HG13	1.96	0.47
1:A:140:GLU:O	1:A:141:ARG:HB2	2.13	0.47
1:B:93:LYS:O	1:B:443:LYS:NZ	2.47	0.47
1:A:498:TYR:HB2	1:A:521:MET:CE	2.45	0.47
1:A:147:GLY:C	1:A:148:LEU:HG	2.35	0.47
1:A:416:ILE:CA	1:A:513:ARG:HE	2.20	0.47
1:A:302:ARG:HD2	1:A:398:GLU:OE1	2.16	0.46
1:B:231:ARG:HD3	1:B:249:PRO:HB3	1.96	0.46
1:B:544:ALA:HB3	1:B:545:PRO:HD3	1.97	0.45
1:A:121:GLU:HG2	1:A:196:ARG:HG2	1.98	0.45
1:A:221:PRO:HG2	6:A:1174:HOH:O	2.16	0.45
1:A:313:MET:HE1	1:A:323:TYR:HB3	1.98	0.45
1:A:284:ALA:O	1:A:350:ARG:NH1	2.50	0.45
1:B:177:GLU:OE2	1:B:179:LYS:HE3	2.17	0.44
1:A:602:MET:HG3	1:A:622:TYR:CD2	2.52	0.44
1:A:140:GLU:O	1:A:141:ARG:CB	2.63	0.44
1:A:389:LEU:H	1:A:389:LEU:HD12	1.83	0.44
1:A:174:TYR:OH	1:A:193:LYS:NZ	2.51	0.44
1:B:63:VAL:HG13	1:B:122:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ALA:HB3	4:A:803:EDO:H22	1.99	0.44
1:A:410:PRO:HB3	1:A:436:GLN:HG3	1.99	0.44
1:B:465:ARG:HG3	1:B:465:ARG:HH11	1.83	0.44
1:B:586:PRO:HG3	1:B:592:TYR:CE2	2.53	0.44
1:A:160:ALA:N	1:A:161:PRO:HD2	2.32	0.43
1:B:309:MET:O	1:B:313:MET:HG3	2.18	0.43
1:B:652:ALA:HB2	3:B:802:ASP:C	2.39	0.43
1:A:293:ILE:HG21	1:A:390:ARG:HG2	2.00	0.43
1:B:404:ILE:HG22	1:B:406:MET:HG2	2.00	0.43
1:B:117:ASN:HA	1:B:118:PRO:HD2	1.93	0.43
1:B:402:MET:HB3	1:B:402:MET:HE3	1.83	0.42
1:B:58:LEU:HD22	1:B:657:MET:HE1	2.01	0.42
1:B:44:GLN:HG3	1:B:660:ARG:HG2	2.01	0.42
1:B:699:ILE:O	1:B:703:PHE:HB3	2.20	0.42
1:B:660:ARG:HD3	6:B:903:HOH:O	2.20	0.42
1:B:468:ALA:HA	1:B:471:GLN:CD	2.40	0.42
1:A:256:VAL:HG21	1:A:657:MET:HE1	2.01	0.42
1:B:422:ASP:C	1:B:424:ALA:H	2.23	0.42
1:B:125:VAL:HG22	1:B:192:LYS:HE2	2.01	0.42
1:A:85:HIS:HA	1:A:88:TYR:HB2	2.01	0.41
1:B:536:ALA:O	1:B:539:VAL:HG12	2.21	0.41
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.80	0.41
1:B:313:MET:HB2	1:B:313:MET:HE2	1.75	0.41
1:A:353:LYS:HA	1:A:353:LYS:HD2	1.89	0.41
1:B:32:ASN:HB2	6:B:959:HOH:O	2.20	0.41
1:B:389:LEU:HD22	1:B:539:VAL:HB	2.03	0.41
1:B:83:ASN:HB2	1:B:86:CYS:SG	2.60	0.41
1:B:461:ARG:HD2	1:B:465:ARG:NH1	2.36	0.41
1:B:369:ILE:HG22	1:B:371:THR:HB	2.03	0.41
1:A:413:ASP:CG	1:A:414:SER:H	2.25	0.40
1:B:76:ASN:HB3	1:B:255:TRP:CH2	2.57	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	702/703 (100%)	673 (96%)	24 (3%)	5 (1%)	22	22
1	B	689/703 (98%)	655 (95%)	29 (4%)	5 (1%)	22	22
All	All	1391/1406 (99%)	1328 (96%)	53 (4%)	10 (1%)	22	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	ILE
1	A	589	VAL
1	B	450	GLU
1	B	452	ASP
1	B	589	VAL
1	A	140	GLU
1	A	147	GLY
1	A	419	HIS
1	B	169	ALA
1	B	423	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	568/583 (97%)	562 (99%)	6 (1%)	73	85
1	B	489/583 (84%)	487 (100%)	2 (0%)	91	96
All	All	1057/1166 (91%)	1049 (99%)	8 (1%)	81	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	63	VAL
1	A	141	ARG

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Mol	Chain	Res	Type
1	A	166	LYS
1	A	309	MET
1	A	527	SER
1	B	21	MET
1	B	69	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN

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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	0.43	0	5,11,13	0.30	0
4	EDO	A	803	-	3,3,3	0.47	0	2,2,2	0.34	0
3	ASP	B	802	-	2,8,8	0.85	0	1,10,10	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ARG	B	801	-	9,10,11	0.80	0	5,11,13	0.34	0
3	ASP	A	802	-	2,8,8	0.47	0	1,10,10	0.43	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	-
4	EDO	A	803	-	-	1/1/1/1	-
3	ASP	B	802	-	-	2/2/8/8	-
2	ARG	B	801	-	-	0/8/9/11	-
3	ASP	A	802	-	-	2/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	ASP	C-CA-CB-CG
4	A	803	EDO	O1-C1-C2-O2
3	A	802	ASP	N-CA-CB-CG
3	A	802	ASP	C-CA-CB-CG
3	B	802	ASP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	EDO	2	0
3	B	802	ASP	1	0
3	A	802	ASP	1	0

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	703/703 (100%)	-0.13	16 (2%) 60 58	32, 53, 81, 105	0
1	B	695/703 (98%)	0.54	94 (13%) 3 2	31, 72, 144, 192	0
All	All	1398/1406 (99%)	0.20	110 (7%) 12 11	31, 58, 128, 192	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	8.1
1	B	416	ILE	7.3
1	B	409	ALA	6.9
1	B	430	LEU	6.9
1	B	517	LEU	6.1
1	B	480	ALA	6.0
1	B	424	ALA	5.4
1	B	432	SER	5.2
1	B	506	GLU	5.1
1	B	493	PHE	5.0
1	B	426	ARG	4.9
1	A	416	ILE	4.6
1	B	485	ALA	4.5
1	B	507	PHE	4.5
1	B	511	PRO	4.4
1	B	510	ASN	4.3
1	B	524	PHE	4.3
1	B	541	ALA	4.3
1	B	141	ARG	4.2
1	A	418	ASP	4.2
1	B	418	ASP	4.2
1	B	452	ASP	4.0
1	B	489	VAL	3.9
1	B	504	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	498	TYR	3.9
1	B	429	GLY	3.9
1	B	417	ALA	3.8
1	A	148	LEU	3.8
1	A	417	ALA	3.8
1	B	484	SER	3.7
1	B	421	ASP	3.7
1	B	439	ALA	3.7
1	B	521	MET	3.6
1	B	420	TRP	3.6
1	B	441	PHE	3.5
1	B	459	LEU	3.5
1	B	562	GLY	3.5
1	B	482	TYR	3.4
1	B	483	GLY	3.3
1	B	144	LYS	3.3
1	B	494	ASP	3.2
1	B	465	ARG	3.2
1	B	463	ALA	3.2
1	B	468	ALA	3.2
1	B	55	GLY	3.2
1	B	422	ASP	3.2
1	B	423	PRO	3.1
1	B	425	ARG	3.1
1	B	487	ALA	3.1
1	B	462	TYR	3.0
1	B	168	ALA	3.0
1	B	248	VAL	3.0
1	B	172	PRO	3.0
1	A	419	HIS	3.0
1	B	490	GLU	2.9
1	B	542	PHE	2.9
1	A	415	ASP	2.8
1	B	238	GLY	2.8
1	B	514	ASP	2.8
1	B	460	THR	2.8
1	A	420	TRP	2.8
1	B	458	LEU	2.8
1	B	445	TYR	2.7
1	B	488	TYR	2.7
1	B	437	PHE	2.7
1	B	539	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	141	ARG	2.7
1	B	419	HIS	2.7
1	B	528	VAL	2.7
1	B	399	GLY	2.7
1	B	497	ILE	2.6
1	B	502	GLU	2.6
1	B	145	PRO	2.6
1	B	246	ASP	2.6
1	B	410	PRO	2.5
1	B	650	GLY	2.5
1	A	719	HIS	2.5
1	B	435	LYS	2.5
1	B	304	ILE	2.5
1	B	404	ILE	2.5
1	B	454	LEU	2.5
1	B	155	TYR	2.4
1	B	143	LYS	2.4
1	B	516	LEU	2.4
1	B	472	PRO	2.4
1	B	142	ILE	2.4
1	B	505	GLU	2.4
1	B	234	ALA	2.3
1	A	146	SER	2.3
1	B	342	TRP	2.3
1	A	423	PRO	2.3
1	B	518	ARG	2.3
1	B	54	ASN	2.3
1	B	456	ILE	2.3
1	B	408	ASN	2.2
1	B	414	SER	2.2
1	B	666	LEU	2.2
1	A	422	ASP	2.2
1	B	173	GLY	2.2
1	B	466	ILE	2.2
1	A	69	CYS	2.1
1	B	436	GLN	2.1
1	A	170	SER	2.1
1	B	478	GLY	2.1
1	B	428	ALA	2.1
1	B	499	ALA	2.0
1	B	540	ALA	2.0
1	A	414	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	512	ASP	2.0
1	B	519	ASP	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
4	EDO	A	803	4/4	0.88	0.42	61,62,64,64	0
3	ASP	A	802	9/9	0.91	0.22	41,46,53,58	0
3	ASP	B	802	9/9	0.94	0.22	40,45,62,68	0
2	ARG	A	801	11/12	0.94	0.26	41,48,60,68	0
5	NA	A	804	1/1	0.96	0.16	60,60,60,60	0
2	ARG	B	801	11/12	0.96	0.22	31,39,46,53	0

6.5 Other polymers (i)

There are no such residues in this entry.