



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:55 PM UTC

PDB ID : 5JXF / pdb_00005jxf
Title : Crystal structure of Flavobacterium psychrophilum DPP11 in complex with dipeptide Arg-Asp
Authors : Bezerra, G.A.; Fedosyuk, S.; Ohara-Nemoto, Y.; Nemoto, T.K.; DjinoVIC-Carugo, K.
Deposited on : 2016-05-13
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

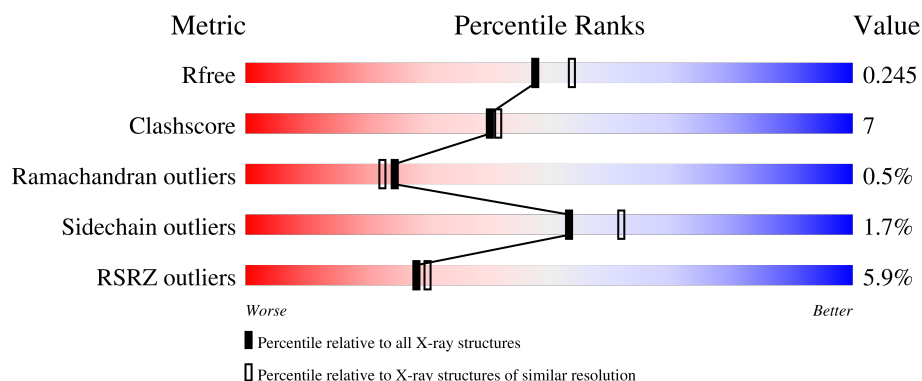
1 Overall quality at a glance

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	731	 4% 80% 13% • 5%
1	B	731	 % 83% 11% 5%
1	C	731	 7% 77% 16% 7%
1	D	731	 10% 76% 16% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22036 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	694	Total	C	N	O	S	0	0	0
			5457	3500	898	1040	19			
1	B	692	Total	C	N	O	S	0	0	0
			5503	3532	910	1042	19			
1	C	682	Total	C	N	O	S	0	0	0
			5272	3380	870	1003	19			
1	D	685	Total	C	N	O	S	0	0	0
			5267	3376	865	1007	19			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A6GWM2
A	-16	GLY	-	expression tag	UNP A6GWM2
A	-15	GLY	-	expression tag	UNP A6GWM2
A	-14	SER	-	expression tag	UNP A6GWM2
A	-13	HIS	-	expression tag	UNP A6GWM2
A	-12	HIS	-	expression tag	UNP A6GWM2
A	-11	HIS	-	expression tag	UNP A6GWM2
A	-10	HIS	-	expression tag	UNP A6GWM2
A	-9	HIS	-	expression tag	UNP A6GWM2
A	-8	HIS	-	expression tag	UNP A6GWM2
A	-7	GLY	-	expression tag	UNP A6GWM2
A	-6	MET	-	expression tag	UNP A6GWM2
A	-5	ALA	-	expression tag	UNP A6GWM2
A	-4	SER	-	expression tag	UNP A6GWM2
A	-3	MET	-	expression tag	UNP A6GWM2
A	-2	THR	-	expression tag	UNP A6GWM2
A	-1	GLY	-	expression tag	UNP A6GWM2
A	0	GLY	-	expression tag	UNP A6GWM2
A	1	GLN	-	expression tag	UNP A6GWM2
A	2	GLN	-	expression tag	UNP A6GWM2
A	3	MET	-	expression tag	UNP A6GWM2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	expression tag	UNP A6GWM2
A	5	ARG	-	expression tag	UNP A6GWM2
A	6	ASP	-	expression tag	UNP A6GWM2
A	7	LEU	-	expression tag	UNP A6GWM2
A	8	TYR	-	expression tag	UNP A6GWM2
A	9	ASP	-	expression tag	UNP A6GWM2
A	10	ASP	-	expression tag	UNP A6GWM2
A	11	ASP	-	expression tag	UNP A6GWM2
A	12	ASP	-	expression tag	UNP A6GWM2
A	13	LYS	-	expression tag	UNP A6GWM2
A	14	ASP	-	expression tag	UNP A6GWM2
A	15	PRO	-	expression tag	UNP A6GWM2
A	16	THR	-	expression tag	UNP A6GWM2
A	17	LEU	-	expression tag	UNP A6GWM2
A	133	ILE	VAL	conflict	UNP A6GWM2
A	442	SER	ALA	conflict	UNP A6GWM2
B	-17	MET	-	initiating methionine	UNP A6GWM2
B	-16	GLY	-	expression tag	UNP A6GWM2
B	-15	GLY	-	expression tag	UNP A6GWM2
B	-14	SER	-	expression tag	UNP A6GWM2
B	-13	HIS	-	expression tag	UNP A6GWM2
B	-12	HIS	-	expression tag	UNP A6GWM2
B	-11	HIS	-	expression tag	UNP A6GWM2
B	-10	HIS	-	expression tag	UNP A6GWM2
B	-9	HIS	-	expression tag	UNP A6GWM2
B	-8	HIS	-	expression tag	UNP A6GWM2
B	-7	GLY	-	expression tag	UNP A6GWM2
B	-6	MET	-	expression tag	UNP A6GWM2
B	-5	ALA	-	expression tag	UNP A6GWM2
B	-4	SER	-	expression tag	UNP A6GWM2
B	-3	MET	-	expression tag	UNP A6GWM2
B	-2	THR	-	expression tag	UNP A6GWM2
B	-1	GLY	-	expression tag	UNP A6GWM2
B	0	GLY	-	expression tag	UNP A6GWM2
B	1	GLN	-	expression tag	UNP A6GWM2
B	2	GLN	-	expression tag	UNP A6GWM2
B	3	MET	-	expression tag	UNP A6GWM2
B	4	GLY	-	expression tag	UNP A6GWM2
B	5	ARG	-	expression tag	UNP A6GWM2
B	6	ASP	-	expression tag	UNP A6GWM2
B	7	LEU	-	expression tag	UNP A6GWM2
B	8	TYR	-	expression tag	UNP A6GWM2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	ASP	-	expression tag	UNP A6GWM2
B	10	ASP	-	expression tag	UNP A6GWM2
B	11	ASP	-	expression tag	UNP A6GWM2
B	12	ASP	-	expression tag	UNP A6GWM2
B	13	LYS	-	expression tag	UNP A6GWM2
B	14	ASP	-	expression tag	UNP A6GWM2
B	15	PRO	-	expression tag	UNP A6GWM2
B	16	THR	-	expression tag	UNP A6GWM2
B	17	LEU	-	expression tag	UNP A6GWM2
B	133	ILE	VAL	conflict	UNP A6GWM2
B	442	SER	ALA	conflict	UNP A6GWM2
C	-17	MET	-	initiating methionine	UNP A6GWM2
C	-16	GLY	-	expression tag	UNP A6GWM2
C	-15	GLY	-	expression tag	UNP A6GWM2
C	-14	SER	-	expression tag	UNP A6GWM2
C	-13	HIS	-	expression tag	UNP A6GWM2
C	-12	HIS	-	expression tag	UNP A6GWM2
C	-11	HIS	-	expression tag	UNP A6GWM2
C	-10	HIS	-	expression tag	UNP A6GWM2
C	-9	HIS	-	expression tag	UNP A6GWM2
C	-8	HIS	-	expression tag	UNP A6GWM2
C	-7	GLY	-	expression tag	UNP A6GWM2
C	-6	MET	-	expression tag	UNP A6GWM2
C	-5	ALA	-	expression tag	UNP A6GWM2
C	-4	SER	-	expression tag	UNP A6GWM2
C	-3	MET	-	expression tag	UNP A6GWM2
C	-2	THR	-	expression tag	UNP A6GWM2
C	-1	GLY	-	expression tag	UNP A6GWM2
C	0	GLY	-	expression tag	UNP A6GWM2
C	1	GLN	-	expression tag	UNP A6GWM2
C	2	GLN	-	expression tag	UNP A6GWM2
C	3	MET	-	expression tag	UNP A6GWM2
C	4	GLY	-	expression tag	UNP A6GWM2
C	5	ARG	-	expression tag	UNP A6GWM2
C	6	ASP	-	expression tag	UNP A6GWM2
C	7	LEU	-	expression tag	UNP A6GWM2
C	8	TYR	-	expression tag	UNP A6GWM2
C	9	ASP	-	expression tag	UNP A6GWM2
C	10	ASP	-	expression tag	UNP A6GWM2
C	11	ASP	-	expression tag	UNP A6GWM2
C	12	ASP	-	expression tag	UNP A6GWM2
C	13	LYS	-	expression tag	UNP A6GWM2

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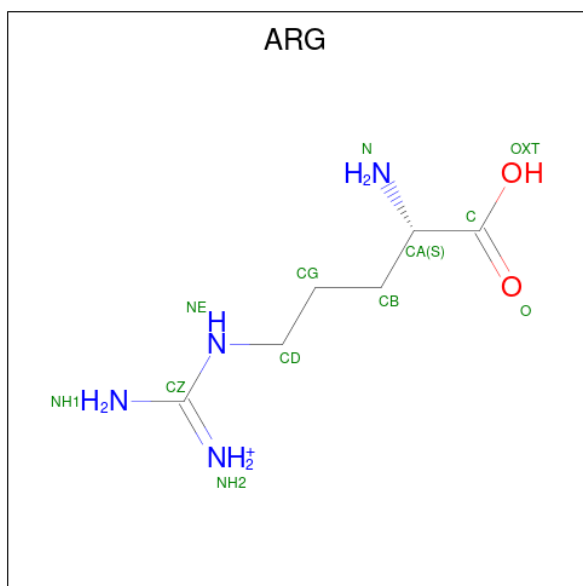
Chain	Residue	Modelled	Actual	Comment	Reference
C	14	ASP	-	expression tag	UNP A6GWM2
C	15	PRO	-	expression tag	UNP A6GWM2
C	16	THR	-	expression tag	UNP A6GWM2
C	17	LEU	-	expression tag	UNP A6GWM2
C	133	ILE	VAL	conflict	UNP A6GWM2
C	442	SER	ALA	conflict	UNP A6GWM2
D	-17	MET	-	initiating methionine	UNP A6GWM2
D	-16	GLY	-	expression tag	UNP A6GWM2
D	-15	GLY	-	expression tag	UNP A6GWM2
D	-14	SER	-	expression tag	UNP A6GWM2
D	-13	HIS	-	expression tag	UNP A6GWM2
D	-12	HIS	-	expression tag	UNP A6GWM2
D	-11	HIS	-	expression tag	UNP A6GWM2
D	-10	HIS	-	expression tag	UNP A6GWM2
D	-9	HIS	-	expression tag	UNP A6GWM2
D	-8	HIS	-	expression tag	UNP A6GWM2
D	-7	GLY	-	expression tag	UNP A6GWM2
D	-6	MET	-	expression tag	UNP A6GWM2
D	-5	ALA	-	expression tag	UNP A6GWM2
D	-4	SER	-	expression tag	UNP A6GWM2
D	-3	MET	-	expression tag	UNP A6GWM2
D	-2	THR	-	expression tag	UNP A6GWM2
D	-1	GLY	-	expression tag	UNP A6GWM2
D	0	GLY	-	expression tag	UNP A6GWM2
D	1	GLN	-	expression tag	UNP A6GWM2
D	2	GLN	-	expression tag	UNP A6GWM2
D	3	MET	-	expression tag	UNP A6GWM2
D	4	GLY	-	expression tag	UNP A6GWM2
D	5	ARG	-	expression tag	UNP A6GWM2
D	6	ASP	-	expression tag	UNP A6GWM2
D	7	LEU	-	expression tag	UNP A6GWM2
D	8	TYR	-	expression tag	UNP A6GWM2
D	9	ASP	-	expression tag	UNP A6GWM2
D	10	ASP	-	expression tag	UNP A6GWM2
D	11	ASP	-	expression tag	UNP A6GWM2
D	12	ASP	-	expression tag	UNP A6GWM2
D	13	LYS	-	expression tag	UNP A6GWM2
D	14	ASP	-	expression tag	UNP A6GWM2
D	15	PRO	-	expression tag	UNP A6GWM2
D	16	THR	-	expression tag	UNP A6GWM2
D	17	LEU	-	expression tag	UNP A6GWM2
D	133	ILE	VAL	conflict	UNP A6GWM2

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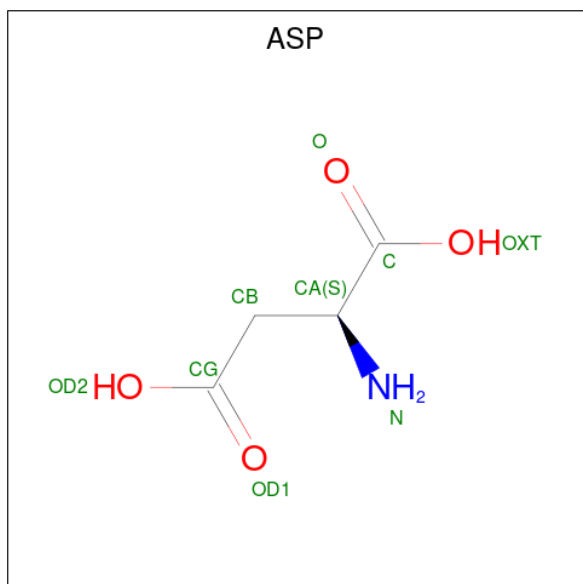
Chain	Residue	Modelled	Actual	Comment	Reference
D	442	SER	ALA	conflict	UNP A6GWM2

- Molecule 2 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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 ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total	O	0	0
			89	89		
6	B	201	Total	O	0	0
			201	201		
6	C	152	Total	O	0	0
			152	152		
6	D	53	Total	O	0	0
			53	53		

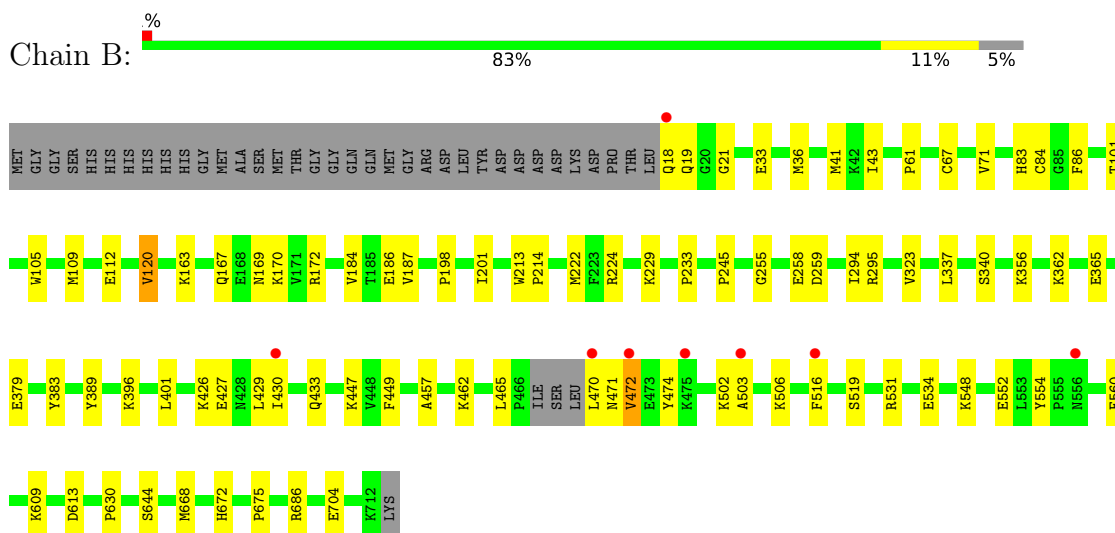
3 Residue-property plots

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.

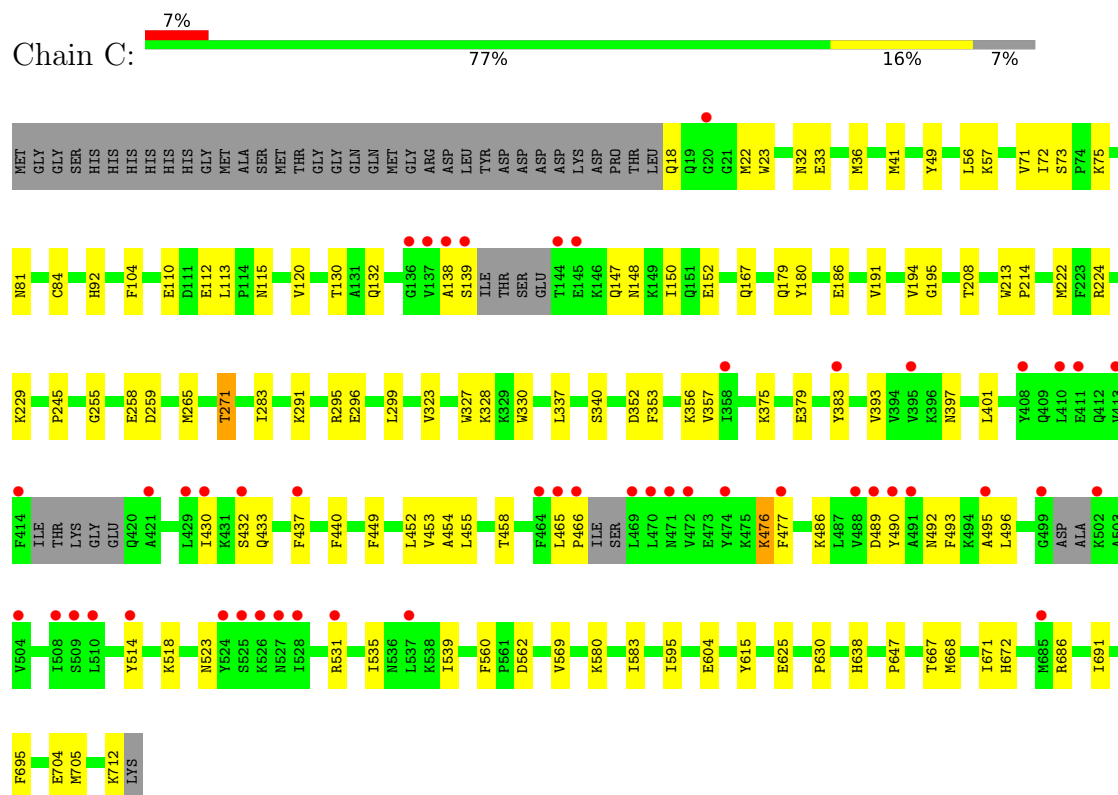
• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase



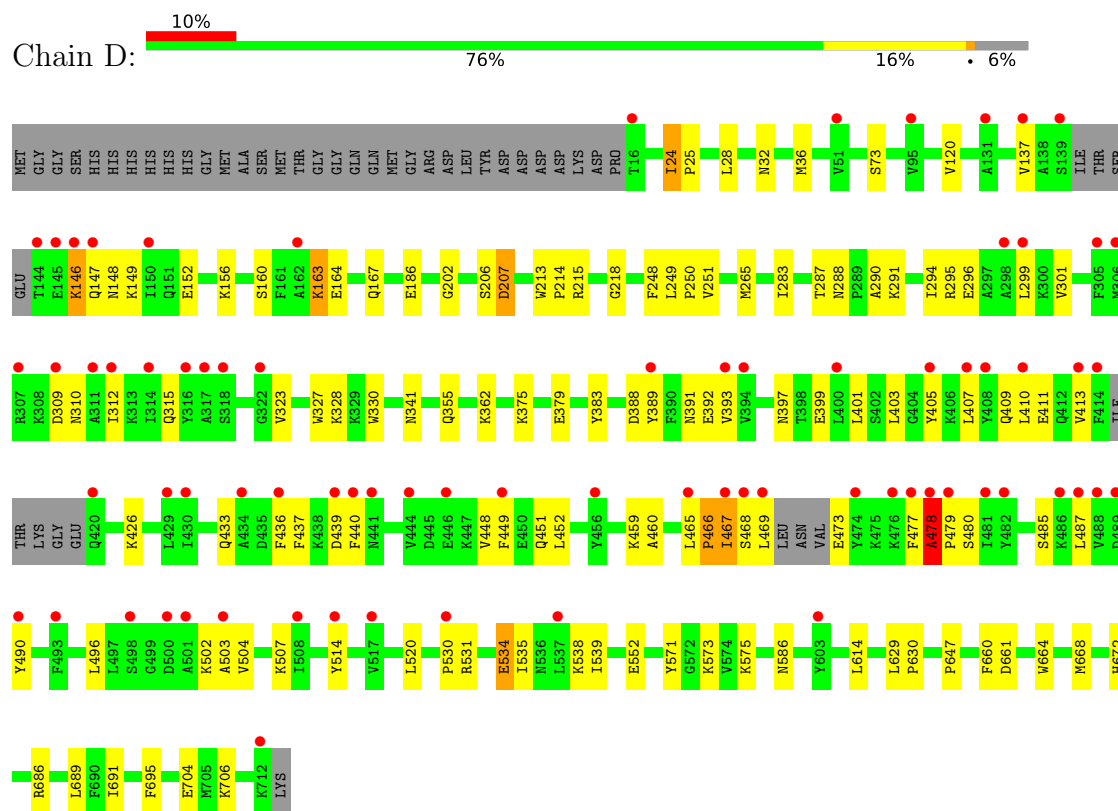
• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase



• 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.05Å 70.69Å 191.60Å 90.00° 97.26° 90.00°	Depositor
Resolution (Å)	46.83 – 2.10 46.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.83-2.10) 98.8 (46.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.244 0.201 , 0.245	Depositor DCC
R_{free} test set	9751 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.3	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	0.96	EDS
Total number of atoms	22036	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, NA

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	0.52	0/5586	0.85	9/7578 (0.1%)
1	B	0.59	0/5631	0.80	0/7621
1	C	0.60	0/5395	0.85	3/7325 (0.0%)
1	D	0.46	0/5390	0.86	8/7326 (0.1%)
All	All	0.55	0/22002	0.84	20/29850 (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
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	ALA	CA-C-N	-10.61	108.59	120.04
1	D	478	ALA	C-N-CA	-10.61	108.59	120.04
1	A	481	ILE	N-CA-C	-7.98	102.14	113.07
1	D	147	GLN	N-CA-C	-7.69	103.62	113.16
1	A	156	LYS	CD-CE-NZ	-7.15	89.02	111.90
1	A	73	SER	CA-C-N	-6.06	114.65	120.83
1	A	73	SER	C-N-CA	-6.06	114.65	120.83
1	A	91	ASN	CA-C-N	-6.04	113.01	122.73
1	A	91	ASN	C-N-CA	-6.04	113.01	122.73
1	C	486	LYS	CD-CE-NZ	-5.87	93.11	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	LYS	CD-CE-NZ	-5.68	93.72	111.90
1	D	586	ASN	CA-C-N	-5.63	115.08	120.83
1	D	586	ASN	C-N-CA	-5.63	115.08	120.83
1	C	113	LEU	CA-C-N	5.60	125.53	119.76
1	C	113	LEU	C-N-CA	5.60	125.53	119.76
1	A	486	LYS	N-CA-C	-5.52	106.42	112.72
1	D	24	ILE	CA-C-N	5.51	126.73	119.84
1	D	24	ILE	C-N-CA	5.51	126.73	119.84
1	A	141	THR	N-CA-C	5.33	122.16	110.80
1	D	413	VAL	N-CA-C	-5.14	104.62	111.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	SER	Peptide
1	D	146	LYS	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	5457	0	5265	67	0
1	B	5503	0	5409	56	0
1	C	5272	0	4980	77	0
1	D	5267	0	4928	78	0
2	A	11	0	12	1	0
2	B	11	0	12	0	0
3	A	8	0	4	1	0
3	B	8	0	4	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	D	1	0	0	0	0
6	A	89	0	0	0	0
6	B	201	0	0	3	0
6	C	152	0	0	3	0
6	D	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22036	0	20614	278	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 (278) 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:C:433:GLN:O	1:C:490:TYR:OH	1.86	0.91
1:A:145:GLU:HA	1:A:148:ASN:HB2	1.56	0.88
1:B:112:GLU:OE2	1:B:224:ARG:NH1	2.10	0.85
1:B:379:GLU:OE2	1:B:531:ARG:NH2	2.12	0.81
1:A:502:LYS:O	1:A:504:VAL:N	2.15	0.79
1:A:319:LYS:NZ	1:A:399:GLU:OE1	2.16	0.79
1:A:373:PHE:CE1	1:A:542:LEU:HB3	2.18	0.79
1:B:668:MET:HE2	1:B:672:HIS:HB3	1.69	0.74
1:B:609:LYS:NZ	1:B:613:ASP:OD2	2.21	0.73
1:C:36:MET:HE3	1:C:41:MET:HE1	1.68	0.73
1:A:215:ARG:NH2	1:A:661:ASP:OD2	2.16	0.73
1:C:295:ARG:HG2	1:C:397:ASN:HD21	1.53	0.73
1:A:28:LEU:HD22	1:A:36:MET:HE1	1.71	0.72
1:C:265:MET:HG2	1:C:569:VAL:HG22	1.72	0.72
1:D:215:ARG:NH2	1:D:661:ASP:OD2	2.20	0.72
1:A:468:SER:OG	1:A:472:VAL:O	2.08	0.71
1:A:486:LYS:HG3	1:A:492:ASN:HB3	1.71	0.71
1:A:276:PRO:HG3	1:A:373:PHE:HD2	1.56	0.70
1:A:373:PHE:HE1	1:A:542:LEU:HB3	1.55	0.69
1:B:337:LEU:HD23	1:B:668:MET:HE3	1.76	0.68
1:D:28:LEU:HD22	1:D:36:MET:HE1	1.77	0.67
1:D:630:PRO:HG3	1:D:686:ARG:CZ	2.25	0.67
1:C:271:THR:HG22	1:C:562:ASP:OD1	1.95	0.66
1:A:36:MET:HE2	1:A:571:TYR:CE1	2.32	0.65
1:C:401:LEU:HD21	1:C:449:PHE:HE2	1.62	0.65
1:A:276:PRO:HG3	1:A:373:PHE:CD2	2.33	0.63
1:B:295:ARG:HD3	1:B:323:VAL:HG13	1.81	0.63
1:C:148:ASN:O	1:C:152:GLU:HG3	1.99	0.62
1:A:668:MET:HE2	1:A:672:HIS:HB3	1.81	0.62
1:D:156:LYS:O	1:D:160:SER:OG	2.18	0.62
1:A:142:SER:O	1:A:144:THR:N	2.32	0.61
1:A:83:HIS:HA	1:A:86:PHE:HB2	1.82	0.61
1:C:437:PHE:CD2	1:C:490:TYR:HE1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:CYS:HG	1:B:84:CYS:HG	1.48	0.60
1:C:430:ILE:C	1:C:432:SER:H	2.10	0.60
1:D:469:LEU:O	1:D:473:GLU:N	2.35	0.60
1:D:401:LEU:HD21	1:D:449:PHE:HE2	1.67	0.60
1:D:290:ALA:HB1	1:D:389:TYR:HE1	1.66	0.60
1:C:73:SER:HB2	1:C:704:GLU:HG2	1.84	0.59
1:C:668:MET:HE2	1:C:672:HIS:HB3	1.85	0.59
1:B:19:GLN:HE21	1:B:675:PRO:HG3	1.68	0.59
1:D:389:TYR:CD2	1:D:460:ALA:HB2	2.37	0.59
1:C:32:ASN:O	1:C:36:MET:HG3	2.03	0.58
1:B:83:HIS:HA	1:B:86:PHE:HB2	1.85	0.58
1:D:299:LEU:HD21	1:D:323:VAL:HG23	1.84	0.58
1:C:138:ALA:O	1:C:139:SER:HB3	2.04	0.58
1:D:437:PHE:CD2	1:D:490:TYR:HB2	2.39	0.58
1:B:383:TYR:CZ	1:B:531:ARG:HG2	2.40	0.57
1:B:33:GLU:HA	1:B:36:MET:HE3	1.86	0.57
1:D:477:PHE:HA	1:D:480:SER:HB3	1.85	0.57
1:A:32:ASN:HB3	1:A:36:MET:HE3	1.87	0.57
1:D:478:ALA:HB3	1:D:479:PRO:HD3	1.86	0.56
1:A:294:ILE:HD11	1:A:389:TYR:CD1	2.40	0.56
1:C:224:ARG:HG2	1:C:224:ARG:HH11	1.71	0.56
1:B:503:ALA:HA	1:B:506:LYS:HB3	1.86	0.56
1:A:167:GLN:HG2	1:A:186:GLU:HG2	1.87	0.56
1:D:36:MET:HE2	1:D:571:TYR:CE2	2.40	0.56
1:B:362:LYS:NZ	1:B:552:GLU:OE2	2.40	0.55
1:D:460:ALA:HB3	1:D:465:LEU:HD11	1.89	0.55
1:C:81:ASN:HB2	1:C:84:CYS:SG	2.47	0.55
1:D:146:LYS:HA	1:D:148:ASN:HB3	1.88	0.55
1:B:462:LYS:HD3	1:B:465:LEU:HD22	1.89	0.55
1:D:290:ALA:HB1	1:D:389:TYR:CE1	2.41	0.55
1:B:105:TRP:HZ3	1:B:222:MET:HE1	1.70	0.55
1:C:337:LEU:HD23	1:C:668:MET:HE3	1.89	0.55
1:C:476:LYS:O	1:C:477:PHE:HB3	2.07	0.55
1:D:466:PRO:O	1:D:468:SER:N	2.40	0.54
1:A:73:SER:HB3	1:A:77:LEU:HB3	1.89	0.54
1:C:295:ARG:HG2	1:C:397:ASN:ND2	2.23	0.54
1:D:301:VAL:HG21	1:D:451:GLN:HG3	1.90	0.54
1:D:393:VAL:HG13	1:D:452:LEU:HB3	1.90	0.54
1:C:75:LYS:O	1:C:224:ARG:HD2	2.08	0.53
1:B:255:GLY:HA3	1:B:686:ARG:CZ	2.39	0.53
1:B:531:ARG:NH1	1:B:534:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:PRO:HG3	1:C:686:ARG:CZ	2.38	0.53
1:A:145:GLU:CA	1:A:148:ASN:HB2	2.36	0.53
1:C:437:PHE:HA	1:C:440:PHE:HB3	1.90	0.53
1:D:407:LEU:HD12	1:D:410:LEU:HD11	1.91	0.53
1:D:146:LYS:CG	1:D:149:LYS:HB2	2.39	0.53
1:D:213:TRP:CD2	1:D:214:PRO:HA	2.44	0.53
1:C:489:ASP:OD1	1:C:492:ASN:N	2.39	0.53
1:C:375:LYS:O	1:C:379:GLU:HG3	2.09	0.52
1:A:141:THR:HG22	1:A:142:SER:N	2.23	0.52
1:C:33:GLU:HA	1:C:36:MET:HE2	1.91	0.52
1:D:32:ASN:HB3	1:D:36:MET:HE3	1.92	0.52
1:C:490:TYR:HA	1:C:493:PHE:HB3	1.91	0.52
1:D:73:SER:HB2	1:D:704:GLU:HG2	1.89	0.52
1:B:429:LEU:O	1:B:433:GLN:HG2	2.09	0.52
1:D:167:GLN:HG2	1:D:186:GLU:HG2	1.91	0.52
1:C:92:HIS:HE1	1:C:115:ASN:OD1	1.92	0.52
1:D:629:LEU:HD12	1:D:630:PRO:HD2	1.90	0.52
1:C:492:ASN:HA	1:C:495:ALA:HB3	1.91	0.52
1:D:411:GLU:OE1	1:D:514:TYR:OH	2.21	0.52
1:C:265:MET:O	1:C:647:PRO:HD2	2.09	0.52
1:B:613:ASP:OD1	6:B:901:HOH:O	2.19	0.51
1:B:401:LEU:HD21	1:B:449:PHE:HE2	1.76	0.51
1:C:531:ARG:O	1:C:535:ILE:HG13	2.11	0.51
1:C:466:PRO:HD2	1:C:523:ASN:ND2	2.26	0.51
1:A:630:PRO:HG2	1:A:686:ARG:CZ	2.40	0.51
1:D:283:ILE:O	1:D:288:ASN:HB2	2.10	0.51
1:D:32:ASN:HB3	1:D:36:MET:CE	2.41	0.51
1:A:337:LEU:HD23	1:A:668:MET:HE3	1.93	0.50
1:B:83:HIS:CE1	1:B:644:SER:HG	2.27	0.50
1:D:291:LYS:HG2	1:D:392:GLU:HG3	1.94	0.50
1:B:356:LYS:HD3	1:B:554:TYR:CZ	2.46	0.50
1:A:284:VAL:HG13	1:A:338:LYS:HE3	1.93	0.50
1:C:535:ILE:O	1:C:539:ILE:HG13	2.11	0.50
1:D:309:ASP:OD1	1:D:310:ASN:N	2.45	0.50
1:C:712:LYS:O	6:C:901:HOH:O	2.18	0.50
1:D:215:ARG:HG2	1:D:660:PHE:CZ	2.47	0.49
1:A:419:GLU:HG3	1:A:501:ALA:CB	2.43	0.49
1:D:296:GLU:HB2	1:D:327:TRP:HE1	1.77	0.49
1:B:21:GLY:HA2	1:B:560:PHE:CD1	2.47	0.49
1:D:379:GLU:CD	1:D:531:ARG:HH22	2.20	0.49
1:B:109:MET:HE2	1:B:224:ARG:CZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:ILE:HG13	1:C:615:TYR:CD2	2.48	0.49
1:B:337:LEU:HD23	1:B:668:MET:CE	2.42	0.49
1:C:255:GLY:HA3	1:C:686:ARG:CZ	2.43	0.49
1:C:258:GLU:O	1:C:259:ASP:HB2	2.12	0.48
1:C:352:ASP:O	1:C:356:LYS:HG3	2.13	0.48
1:C:437:PHE:CE1	1:C:440:PHE:CD2	3.01	0.48
1:C:466:PRO:HD2	1:C:523:ASN:HD21	1.78	0.48
1:A:271:THR:HG22	1:A:562:ASP:OD1	2.12	0.48
1:B:365:GLU:OE2	1:B:548:LYS:NZ	2.40	0.48
1:C:112:GLU:HG2	1:C:194:VAL:HG22	1.94	0.48
1:D:362:LYS:HE2	1:D:552:GLU:OE2	2.14	0.48
1:D:383:TYR:OH	1:D:531:ARG:HD3	2.13	0.48
1:D:668:MET:HE2	1:D:672:HIS:HB3	1.94	0.48
1:B:109:MET:HE2	1:B:224:ARG:NE	2.28	0.48
1:C:49:TYR:CD2	1:C:57:LYS:HD3	2.49	0.48
1:D:283:ILE:HA	1:D:287:THR:OG1	2.14	0.48
1:A:298:ALA:HA	1:A:448:VAL:HG23	1.96	0.48
1:C:167:GLN:HG2	1:C:186:GLU:HG2	1.95	0.48
1:A:32:ASN:O	1:A:36:MET:HG3	2.13	0.47
1:A:486:LYS:HG2	1:A:496:LEU:HB2	1.96	0.47
1:C:401:LEU:HD21	1:C:449:PHE:CE2	2.45	0.47
1:B:294:ILE:HD11	1:B:389:TYR:CD1	2.50	0.47
1:D:433:GLN:HB3	1:D:436:PHE:CD2	2.49	0.47
1:D:496:LEU:HD12	1:D:507:LYS:HG2	1.96	0.47
1:A:99:TYR:CD1	1:A:104:PHE:HB2	2.50	0.47
1:B:198:PRO:HD2	1:B:201:ILE:HD12	1.96	0.47
1:C:295:ARG:HD2	1:C:330:TRP:HZ3	1.78	0.47
1:A:129:VAL:O	1:A:133:ILE:HG12	2.15	0.47
1:A:416:THR:HG22	1:A:417:LYS:HG2	1.96	0.47
1:A:615:TYR:O	1:A:618:LYS:NZ	2.36	0.47
1:B:340:SER:OG	1:B:668:MET:HE1	2.14	0.47
1:D:215:ARG:HG2	1:D:660:PHE:HZ	1.80	0.47
1:D:265:MET:O	1:D:647:PRO:HD2	2.14	0.47
1:D:573:LYS:HE3	1:D:575:LYS:HD3	1.97	0.47
1:D:691:ILE:O	1:D:695:PHE:HB3	2.15	0.46
1:A:148:ASN:O	1:A:152:GLU:HG3	2.15	0.46
1:B:224:ARG:NH2	1:B:704:GLU:OE1	2.48	0.46
1:C:208:THR:OG1	1:C:604:GLU:OE2	2.28	0.46
1:C:492:ASN:O	1:C:496:LEU:HB2	2.15	0.46
1:A:419:GLU:HG3	1:A:501:ALA:HB2	1.97	0.46
1:A:644:SER:OG	3:A:802:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:TYR:OH	1:C:518:LYS:HE3	2.16	0.46
1:D:202:GLY:HA2	1:D:218:GLY:O	2.16	0.46
1:D:448:VAL:HG13	1:D:452:LEU:HD22	1.98	0.46
1:C:299:LEU:HD21	1:C:323:VAL:HB	1.97	0.46
1:C:691:ILE:O	1:C:695:PHE:HB3	2.16	0.46
1:A:81:ASN:HB2	1:A:84:CYS:SG	2.56	0.46
1:A:213:TRP:CD2	1:A:214:PRO:HA	2.51	0.46
1:C:120:VAL:HG23	1:C:191:VAL:HG21	1.97	0.46
1:C:110:GLU:OE1	1:C:110:GLU:N	2.34	0.45
1:D:388:ASP:HA	1:D:391:ASN:HB2	1.98	0.45
1:D:403:LEU:HD22	1:D:436:PHE:HZ	1.82	0.45
1:D:436:PHE:O	1:D:440:PHE:HB2	2.17	0.45
1:A:31:MET:HE2	1:A:31:MET:HB3	1.88	0.45
1:A:502:LYS:O	1:A:505:LEU:N	2.46	0.45
1:B:457:ALA:HA	1:B:471:ASN:HD22	1.82	0.45
1:D:328:LYS:HB3	1:D:664:TRP:HZ3	1.82	0.45
1:C:112:GLU:CD	1:C:194:VAL:HG22	2.43	0.44
1:A:391:ASN:O	1:A:396:LYS:HG3	2.17	0.44
1:B:71:VAL:HG11	1:B:245:PRO:HG3	1.99	0.44
1:C:283:ILE:HD13	1:C:671:ILE:HD11	1.99	0.44
1:C:340:SER:OG	1:C:668:MET:HE1	2.18	0.44
1:B:213:TRP:CD2	1:B:214:PRO:HA	2.52	0.44
1:C:132:GLN:HG3	6:C:1016:HOH:O	2.18	0.44
1:B:167:GLN:HG2	1:B:186:GLU:HG2	1.98	0.44
1:C:454:ALA:O	1:C:458:THR:HG22	2.17	0.44
1:A:142:SER:O	1:A:142:SER:OG	2.30	0.44
1:A:271:THR:HB	1:A:563:ALA:H	1.82	0.44
1:C:514:TYR:CZ	1:C:518:LYS:HE3	2.53	0.44
1:D:164:GLU:HB2	1:D:167:GLN:CD	2.43	0.44
1:D:502:LYS:C	1:D:504:VAL:H	2.25	0.44
1:A:354:GLN:HA	1:A:357:VAL:HG13	1.99	0.44
1:B:447:LYS:HE3	1:B:447:LYS:HB3	1.82	0.44
1:D:315:GLN:HE21	1:D:439:ASP:C	2.26	0.44
1:A:283:ILE:HA	1:A:287:THR:OG1	2.18	0.44
1:B:470:LEU:C	1:B:472:VAL:H	2.26	0.43
1:D:251:VAL:HG11	1:D:689:LEU:HD11	2.00	0.43
1:A:71:VAL:HG11	1:A:245:PRO:HG3	1.98	0.43
1:A:213:TRP:HB2	1:A:663:VAL:HG12	2.00	0.43
1:A:210:ASN:OD1	2:A:801:ARG:N	2.51	0.43
1:B:18:GLN:HG3	1:B:19:GLN:N	2.33	0.43
1:B:630:PRO:HG3	1:B:686:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HD12	1:C:705:MET:HE2	2.00	0.43
1:D:295:ARG:HG2	1:D:397:ASN:OD1	2.17	0.43
1:B:187:VAL:O	1:B:233:PRO:HB3	2.19	0.43
1:D:392:GLU:O	1:D:397:ASN:HB2	2.19	0.43
1:B:33:GLU:HA	1:B:36:MET:CE	2.47	0.43
1:B:465:LEU:HD12	1:B:465:LEU:HA	1.92	0.43
1:D:389:TYR:HD2	1:D:460:ALA:HB2	1.84	0.43
1:D:466:PRO:HG2	1:D:520:LEU:HD22	2.01	0.43
1:D:531:ARG:NH1	1:D:535:ILE:HD11	2.34	0.43
1:A:518:LYS:HB3	1:A:518:LYS:HE2	1.84	0.42
1:B:101:THR:O	1:B:198:PRO:HB3	2.19	0.42
1:D:149:LYS:O	1:D:152:GLU:HB2	2.19	0.42
1:D:405:TYR:O	1:D:409:GLN:HG2	2.19	0.42
1:A:479:PRO:HG2	1:A:480:SER:H	1.84	0.42
1:C:72:ILE:HD11	1:C:222:MET:HE2	2.01	0.42
1:D:466:PRO:HB2	1:D:467:ILE:H	1.59	0.42
1:A:277:SER:N	1:A:350:GLU:OE2	2.50	0.42
1:B:163:LYS:NZ	6:B:921:HOH:O	2.51	0.42
1:B:470:LEU:O	1:B:471:ASN:HB2	2.18	0.42
1:C:22:MET:HE3	1:C:638:HIS:CD2	2.55	0.42
1:C:295:ARG:HD2	1:C:330:TRP:CZ3	2.53	0.42
1:D:534:GLU:O	1:D:538:LYS:HD3	2.19	0.42
1:C:455:LEU:HD12	1:C:455:LEU:HA	1.91	0.42
1:D:485:SER:C	1:D:487:LEU:H	2.27	0.42
1:B:222:MET:HE3	1:B:222:MET:HB2	1.74	0.42
1:D:28:LEU:O	1:D:32:ASN:HB2	2.20	0.42
1:D:295:ARG:HD2	1:D:330:TRP:CZ3	2.54	0.42
1:B:516:PHE:O	1:B:519:SER:HB3	2.19	0.42
1:A:382:PRO:HB2	1:A:464:PHE:HE2	1.84	0.42
1:A:489:ASP:HB3	1:A:492:ASN:HB2	2.01	0.42
1:C:104:PHE:O	1:C:195:GLY:HA2	2.19	0.42
1:D:291:LYS:HB3	1:D:330:TRP:CZ3	2.55	0.42
1:A:702:ILE:HA	1:A:705:MET:HE3	2.02	0.42
1:B:61:PRO:HB2	1:B:120:VAL:HG13	2.02	0.42
1:A:340:SER:OG	1:A:668:MET:HE1	2.19	0.42
1:B:426:LYS:O	1:B:430:ILE:HG13	2.20	0.42
1:C:328:LYS:NZ	6:C:910:HOH:O	2.52	0.42
1:C:353:PHE:O	1:C:357:VAL:HG23	2.20	0.42
1:D:163:LYS:HE3	1:D:167:GLN:O	2.20	0.42
1:B:33:GLU:OE1	6:B:902:HOH:O	2.22	0.42
1:A:489:ASP:HB3	1:A:492:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:MET:HE3	1:B:43:ILE:O	2.20	0.41
1:B:170:LYS:HZ2	1:B:172:ARG:HD3	1.85	0.41
1:D:614:LEU:HD23	1:D:614:LEU:HA	1.90	0.41
1:A:466:PRO:HB2	1:A:467:ILE:H	1.62	0.41
1:A:512:LYS:HD2	1:A:512:LYS:HA	1.71	0.41
1:C:291:LYS:HB3	1:C:330:TRP:CZ3	2.55	0.41
1:C:449:PHE:CZ	1:C:453:VAL:HG21	2.55	0.41
1:D:294:ILE:HD13	1:D:393:VAL:HG23	2.03	0.41
1:A:478:ALA:O	1:A:481:ILE:HG13	2.20	0.41
1:D:503:ALA:O	1:D:507:LYS:N	2.52	0.41
1:A:24:ILE:HA	1:A:25:PRO:HD3	1.87	0.41
1:C:71:VAL:HG11	1:C:245:PRO:HG3	2.03	0.41
1:A:265:MET:O	1:A:647:PRO:HD2	2.20	0.41
1:A:490:TYR:CZ	1:A:494:LYS:HE3	2.55	0.41
1:A:215:ARG:HG2	1:A:660:PHE:HZ	1.85	0.41
1:C:150:ILE:HD13	1:C:180:TYR:OH	2.21	0.41
1:C:580:LYS:HE3	1:C:583:ILE:HD12	2.02	0.41
1:A:429:LEU:O	1:A:433:GLN:HG2	2.20	0.41
1:A:383:TYR:CZ	1:A:531:ARG:HG2	2.56	0.41
1:B:258:GLU:O	1:B:259:ASP:HB2	2.19	0.41
1:D:207:ASP:O	1:D:328:LYS:NZ	2.52	0.41
1:D:535:ILE:O	1:D:539:ILE:HG13	2.21	0.41
1:B:169:ASN:OD1	1:B:184:VAL:HG22	2.21	0.41
1:D:24:ILE:HA	1:D:25:PRO:HD3	1.83	0.41
1:D:249:LEU:HA	1:D:250:PRO:HD3	1.97	0.41
1:C:23:TRP:CZ3	1:C:560:PHE:HB3	2.56	0.40
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.92	0.40
1:C:383:TYR:CE2	1:C:531:ARG:HB2	2.56	0.40
1:C:393:VAL:HG13	1:C:452:LEU:HB3	2.02	0.40
1:D:403:LEU:HD23	1:D:487:LEU:HB3	2.03	0.40
1:B:502:LYS:O	1:B:503:ALA:HB3	2.21	0.40
1:C:33:GLU:HA	1:C:36:MET:CE	2.50	0.40
1:D:248:PHE:CZ	1:D:706:LYS:HE2	2.56	0.40
1:C:213:TRP:CD2	1:C:214:PRO:HA	2.57	0.40
1:C:296:GLU:HB2	1:C:327:TRP:NE1	2.36	0.40
1:D:433:GLN:HB3	1:D:436:PHE:CE2	2.56	0.40
1:A:32:ASN:HB3	1:A:36:MET:CE	2.50	0.40
1:A:408:TYR:O	1:A:411:GLU:HB3	2.21	0.40
1:B:83:HIS:CE1	1:B:644:SER:OG	2.75	0.40
1:C:130:THR:OG1	1:C:179:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	690/731 (94%)	647 (94%)	37 (5%)	6 (1%)	14	10
1	B	688/731 (94%)	662 (96%)	25 (4%)	1 (0%)	48	50
1	C	672/731 (92%)	641 (95%)	29 (4%)	2 (0%)	36	36
1	D	677/731 (93%)	633 (94%)	40 (6%)	4 (1%)	21	18
All	All	2727/2924 (93%)	2583 (95%)	131 (5%)	13 (0%)	24	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	502	LYS
1	A	503	ALA
1	D	206	SER
1	D	467	ILE
1	A	466	PRO
1	A	480	SER
1	D	466	PRO
1	A	479	PRO
1	C	476	LYS
1	D	478	ALA
1	B	474	TYR
1	C	465	LEU

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	577/631 (91%)	564 (98%)	13 (2%)	44	51
1	B	593/631 (94%)	588 (99%)	5 (1%)	73	81
1	C	538/631 (85%)	532 (99%)	6 (1%)	65	74
1	D	530/631 (84%)	517 (98%)	13 (2%)	42	48
All	All	2238/2524 (89%)	2201 (98%)	37 (2%)	53	62

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	62	HIS
1	A	73	SER
1	A	92	HIS
1	A	137	VAL
1	A	144	THR
1	A	148	ASN
1	A	160	SER
1	A	271	THR
1	A	286	GLU
1	A	358	ILE
1	A	486	LYS
1	A	512	LYS
1	B	120	VAL
1	B	229	LYS
1	B	396	LYS
1	B	427	GLU
1	B	472	VAL
1	C	18	GLN
1	C	147	GLN
1	C	229	LYS
1	C	271	THR
1	C	625	GLU
1	C	667	THR
1	D	120	VAL
1	D	137	VAL
1	D	163	LYS
1	D	207	ASP
1	D	312	ILE
1	D	341	ASN
1	D	355	GLN
1	D	375	LYS
1	D	399	GLU

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Mol	Chain	Res	Type
1	D	426	LYS
1	D	459	LYS
1	D	530	PRO
1	D	534	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	38	ASN
1	A	81	ASN
1	A	127	ASN
1	A	451	GLN
1	A	637	ASN
1	A	680	ASN
1	B	19	GLN
1	B	32	ASN
1	B	62	HIS
1	B	132	GLN
1	B	433	GLN
1	B	471	ASN
1	B	637	ASN
1	C	19	GLN
1	C	62	HIS
1	C	92	HIS
1	C	117	ASN
1	C	127	ASN
1	C	132	GLN
1	C	232	HIS
1	C	282	GLN
1	C	302	GLN
1	C	397	ASN
1	C	423	ASN
1	C	523	ASN
1	C	637	ASN
1	C	638	HIS
1	D	62	HIS
1	D	282	GLN
1	D	288	ASN
1	D	637	ASN
1	D	654	ASN
1	D	672	HIS

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Mol	Chain	Res	Type
1	D	680	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 8 ligands modelled in this entry, 4 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	$\# Z > 2$
3	ASP	A	802	-	6,7,8	0.90	0	4,8,10	1.09	0
2	ARG	B	801	-	9,10,11	0.51	0	5,11,13	0.24	0
2	ARG	A	801	-	9,10,11	0.47	0	5,11,13	0.28	0
3	ASP	B	802	-	6,7,8	1.13	0	4,8,10	1.21	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
3	ASP	A	802	-	-	2/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	B	801	-	-	0/8/9/11	-
2	ARG	A	801	-	-	0/8/9/11	-
3	ASP	B	802	-	-	3/5/6/8	-

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	A	802	ASP	C-CA-CB-CG
3	B	802	ASP	O-C-CA-CB
3	B	802	ASP	C-CA-CB-CG
3	A	802	ASP	N-CA-CB-CG
3	B	802	ASP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ASP	1	0
2	A	801	ARG	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	694/731 (94%)	0.44	31 (4%) 38 40	35, 66, 106, 139	0
1	B	692/731 (94%)	0.06	8 (1%) 76 78	28, 50, 80, 99	0
1	C	682/731 (93%)	0.41	49 (7%) 21 23	28, 58, 108, 124	0
1	D	685/731 (93%)	0.82	75 (10%) 10 11	44, 73, 126, 143	0
All	All	2753/2924 (94%)	0.43	163 (5%) 28 30	28, 62, 112, 143	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	414	PHE	6.8
1	A	501	ALA	5.2
1	C	528	ILE	5.0
1	D	456	TYR	4.8
1	C	491	ALA	4.7
1	D	487	LEU	4.7
1	A	478	ALA	4.6
1	D	467	ILE	4.6
1	C	469	LEU	4.5
1	A	472	VAL	4.5
1	A	467	ILE	4.5
1	A	140	ILE	4.4
1	D	314	ILE	4.4
1	C	490	TYR	4.3
1	D	316	TYR	4.3
1	C	437	PHE	4.3
1	B	470	LEU	4.2
1	C	138	ALA	4.1
1	D	603	TYR	4.1
1	D	482	TYR	3.9
1	D	501	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	488	VAL	3.9
1	D	436	PHE	3.9
1	C	509	SER	3.8
1	C	137	VAL	3.8
1	B	503	ALA	3.7
1	D	131	ALA	3.7
1	D	478	ALA	3.7
1	D	312	ILE	3.7
1	C	474	TYR	3.6
1	D	469	LEU	3.6
1	A	367	GLY	3.5
1	D	474	TYR	3.5
1	D	508	ILE	3.5
1	C	414	PHE	3.5
1	C	20	GLY	3.5
1	A	477	PHE	3.4
1	D	489	ASP	3.4
1	C	139	SER	3.3
1	D	305	PHE	3.3
1	A	468	SER	3.3
1	C	410	LEU	3.3
1	A	474	TYR	3.2
1	A	141	THR	3.2
1	C	466	PRO	3.2
1	D	477	PHE	3.2
1	C	465	LEU	3.1
1	A	144	THR	3.1
1	A	481	ILE	3.1
1	D	446	GLU	3.1
1	D	479	PRO	3.1
1	B	475	LYS	3.1
1	B	18	GLN	3.1
1	D	449	PHE	3.1
1	C	489	ASP	3.1
1	A	479	PRO	3.0
1	C	136	GLY	3.0
1	C	471	ASN	3.0
1	D	490	TYR	3.0
1	D	430	ILE	3.0
1	D	394	VAL	3.0
1	D	429	LEU	3.0
1	C	144	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	514	TYR	3.0
1	D	139	SER	2.9
1	D	476	LYS	2.9
1	A	373	PHE	2.9
1	D	389	TYR	2.9
1	C	524	TYR	2.9
1	D	440	PHE	2.9
1	C	413	VAL	2.8
1	C	472	VAL	2.8
1	D	413	VAL	2.8
1	C	526	LYS	2.8
1	D	468	SER	2.8
1	A	358	ILE	2.8
1	D	439	ASP	2.8
1	D	503	ALA	2.8
1	A	416	THR	2.8
1	D	517	VAL	2.8
1	D	444	VAL	2.7
1	C	464	PHE	2.6
1	D	500	ASP	2.6
1	B	516	PHE	2.6
1	C	470	LEU	2.6
1	C	429	LEU	2.6
1	A	143	GLU	2.6
1	D	486	LYS	2.6
1	C	537	LEU	2.6
1	D	393	VAL	2.5
1	D	145	GLU	2.5
1	C	395	VAL	2.5
1	B	556	ASN	2.5
1	C	145	GLU	2.5
1	A	525	SER	2.5
1	D	16	THR	2.5
1	D	712	LYS	2.5
1	A	207	ASP	2.4
1	D	144	THR	2.4
1	D	407	LEU	2.4
1	D	420	GLN	2.4
1	D	493	PHE	2.4
1	C	685	MET	2.4
1	D	146	LYS	2.4
1	D	299	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	556	ASN	2.4
1	B	430	ILE	2.4
1	D	498	SER	2.4
1	D	408	TYR	2.3
1	D	317	ALA	2.3
1	C	527	ASN	2.3
1	C	525	SER	2.3
1	D	147	GLN	2.3
1	C	510	LEU	2.3
1	D	307	ARG	2.3
1	A	512	LYS	2.3
1	C	430	ILE	2.3
1	B	472	VAL	2.3
1	D	137	VAL	2.3
1	D	441	ASN	2.3
1	A	482	TYR	2.3
1	D	309	ASP	2.3
1	A	505	LEU	2.3
1	C	358	ILE	2.2
1	C	508	ILE	2.2
1	D	530	PRO	2.2
1	C	495	ALA	2.2
1	D	162	ALA	2.2
1	C	488	VAL	2.2
1	D	51	VAL	2.2
1	A	136	GLY	2.2
1	C	499	GLY	2.2
1	A	359	ALA	2.2
1	A	496	LEU	2.2
1	D	465	LEU	2.2
1	C	383	TYR	2.2
1	D	514	TYR	2.2
1	C	504	VAL	2.2
1	C	411	GLU	2.2
1	C	477	PHE	2.1
1	D	537	LEU	2.1
1	A	351	LYS	2.1
1	C	531	ARG	2.1
1	D	95	VAL	2.1
1	A	712	LYS	2.1
1	C	421	ALA	2.1
1	D	434	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	400	LEU	2.1
1	D	322	GLY	2.1
1	D	150	ILE	2.1
1	D	481	ILE	2.1
1	C	432	SER	2.1
1	D	306	MET	2.0
1	C	502	LYS	2.0
1	A	453	VAL	2.0
1	D	318	SER	2.0
1	D	298	ALA	2.0
1	D	311	ALA	2.0
1	D	410	LEU	2.0
1	A	156	LYS	2.0
1	A	456	TYR	2.0
1	C	408	TYR	2.0
1	D	405	TYR	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(Å ²)	Q<0.9
5	NA	D	803	1/1	0.88	0.12	57,57,57,57	0
3	ASP	A	802	8/9	0.90	0.29	92,106,138,159	0
2	ARG	A	801	11/12	0.90	0.15	60,69,82,82	0
3	ASP	B	802	8/9	0.93	0.11	35,44,61,68	8
4	CL	D	801	1/1	0.95	0.07	81,81,81,81	0
2	ARG	B	801	11/12	0.95	0.09	33,44,57,60	0
4	CL	C	801	1/1	0.96	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	D	802	1/1	0.98	0.05	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.