Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 07:28 PM EDT

PDB ID	:	5JXF
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 (i) 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 (i)) were used in the production of this report:

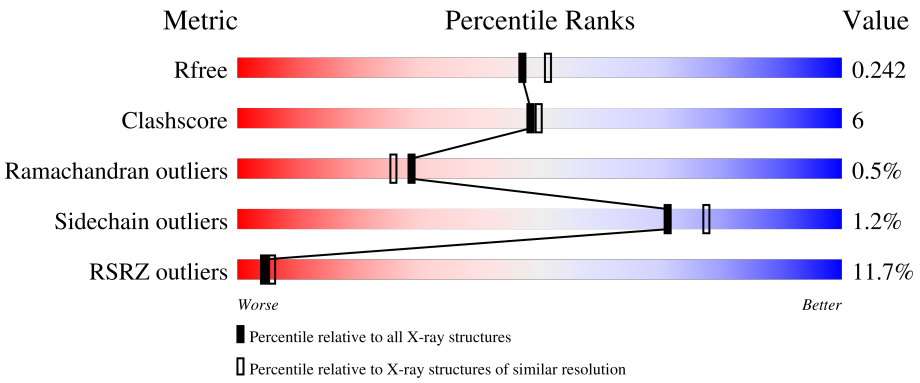
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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}	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 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 <=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	11% 80% 13% • 5%
1	B	731	3% 84% 11% 5%
1	C	731	11% 78% 15% 7%
1	D	731	18% 79% 14% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASP	A	802	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	694	5457	3500	898	1040	19	0	0	0
1	B	692	5503	3532	910	1042	19	0	0	0
1	C	682	5272	3380	870	1003	19	0	0	0
1	D	685	5267	3376	865	1007	19	0	0	0

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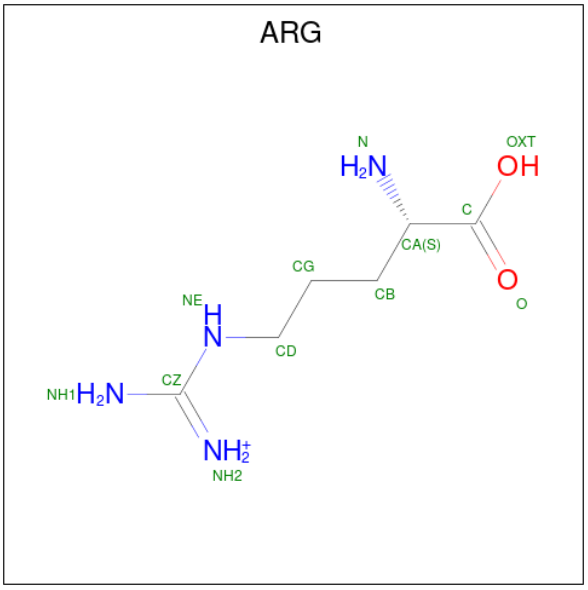
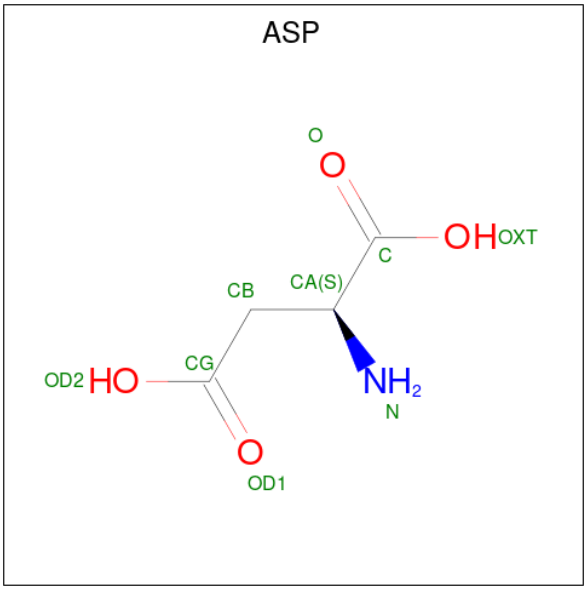
Chain	Residue	Modelled	Actual	Comment	Reference
D	442	SER	ALA	conflict	UNP A6GWM2

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	6	4	1	0	0
			Total	C	N	O		
2	B	1	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
			Total	C	N	O		
3	A	1	8	4	1	3	0	0
3	B	1	8	4	1	3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 6 is water.

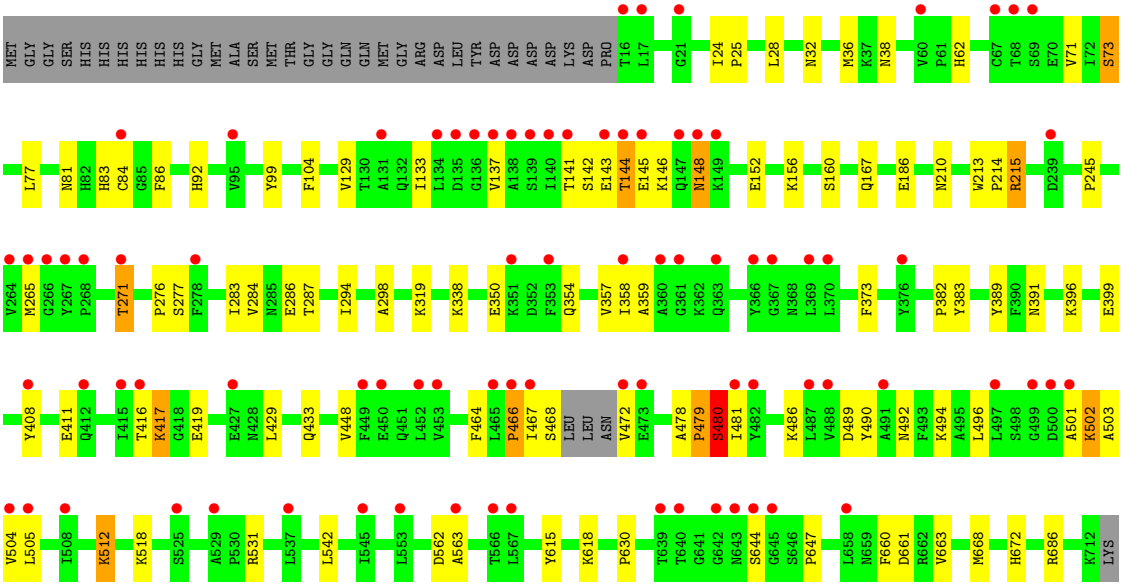
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	89	89	89	0	0
6	B	201	201	201	0	0
6	C	152	152	152	0	0
6	D	53	53	53	0	0

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.

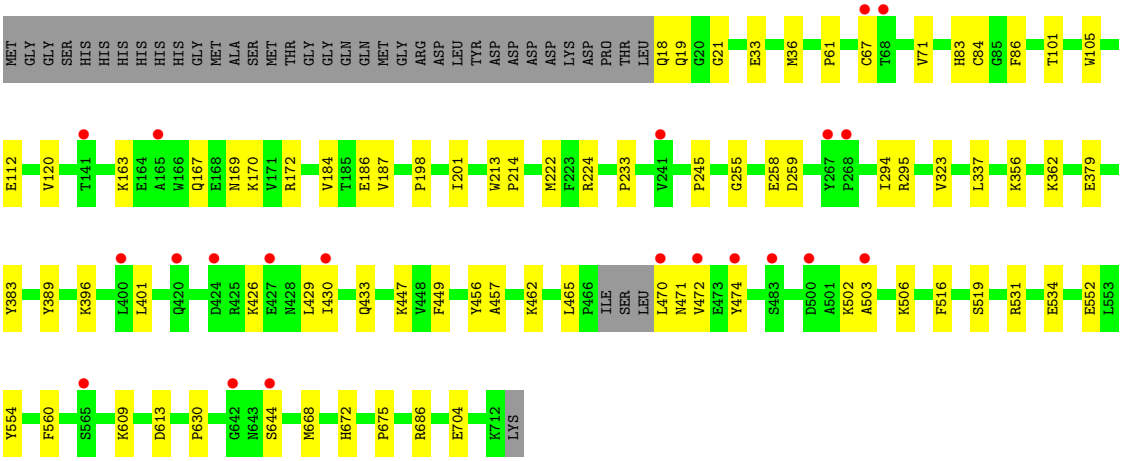
• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase

Chain A:



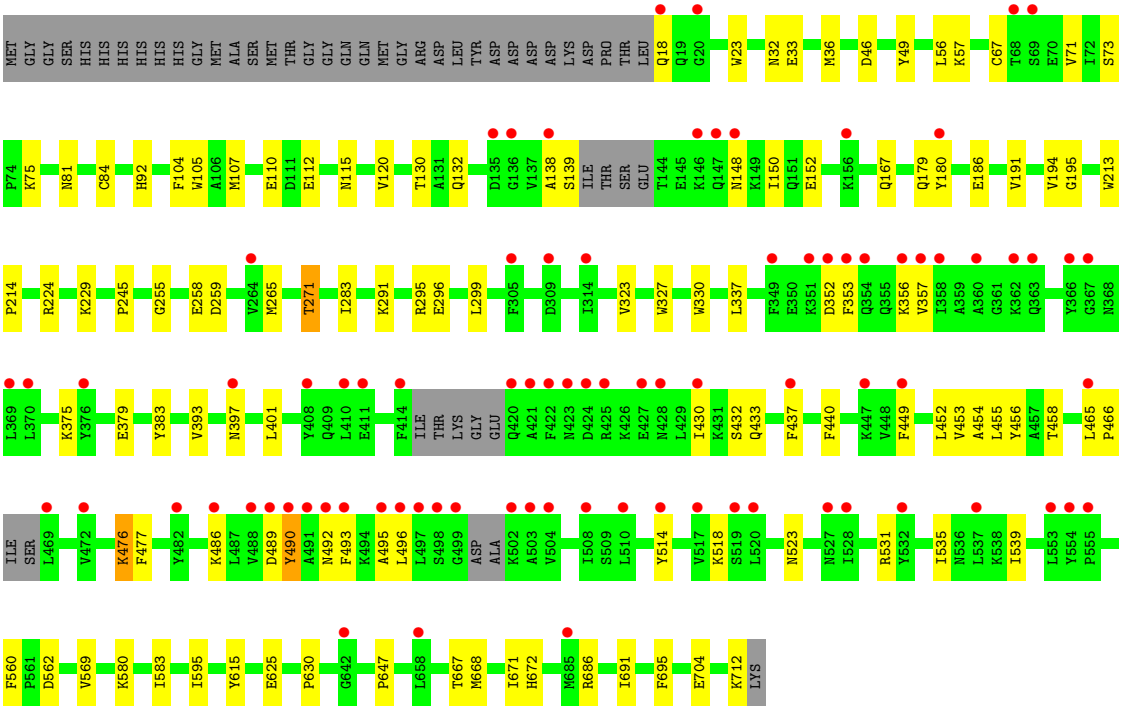
• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase

Chain B:



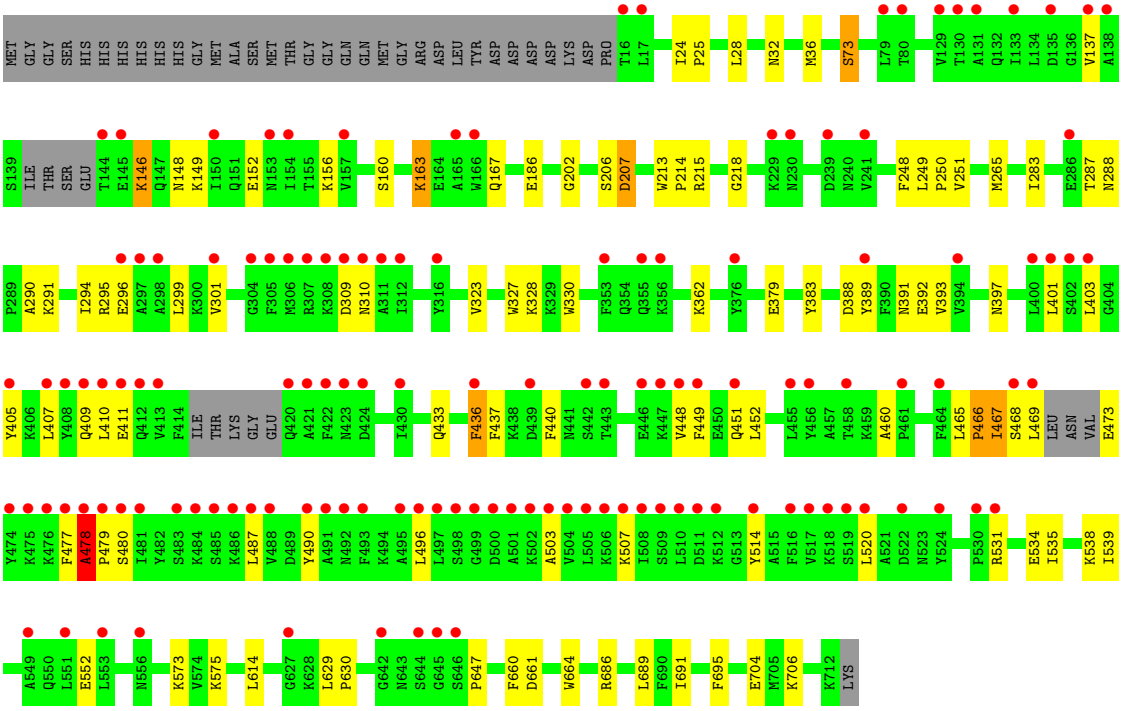
• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.80 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.244 0.198 , 0.242	Depositor DCC
R_{free} test set	9751 reflections (5.04%)	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 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[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: NA, 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	0/5586	0.58	3/7578 (0.0%)
1	B	0.48	0/5631	0.56	0/7621
1	C	0.50	1/5395 (0.0%)	0.59	3/7325 (0.0%)
1	D	0.37	0/5390	0.53	1/7326 (0.0%)
All	All	0.45	1/22002 (0.0%)	0.56	7/29850 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	490	TYR	CG-CD1	-5.79	1.31	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	LYS	CD-CE-NZ	-9.86	89.02	111.70
1	C	486	LYS	CD-CE-NZ	-8.08	93.11	111.70
1	A	417	LYS	CD-CE-NZ	-7.82	93.72	111.70
1	C	490	TYR	CB-CG-CD1	-7.33	116.61	121.00
1	A	215	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	C	490	TYR	CB-CG-CD2	5.33	124.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	478	ALA	C-N-CD	5.13	139.17	128.40

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 (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	5457	0	5265	62	0
1	B	5503	0	5409	50	0
1	C	5272	0	4980	71	0
1	D	5267	0	4928	71	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	2	0
6	D	53	0	0	0	0
All	All	22036	0	20614	254	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 (254) 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:373:PHE:CE1	1:A:542:LEU:HB3	2.18	0.79
1:A:319:LYS:NZ	1:A:399:GLU:OE1	2.16	0.73
1:B:609:LYS:NZ	1:B:613:ASP:OD2	2.21	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: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: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: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: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
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: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:B:668:MET:HE2	1:B:672:HIS:HB3	1.84	0.58
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:33:GLU:HA	1:C:36:MET:HE3	1.86	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:D:477:PHE:HA	1:D:480:SER:HB3	1.85	0.57
1:D:478:ALA:HB3	1:D:479:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:430:ILE:C	1:C:432:SER:H	2.10	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: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
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:B:337:LEU:HA	1:B:668:MET:HE3	1.90	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: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:67:CYS:HG	1:B:84:CYS:HG	1.54	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:B:337:LEU:HD23	1:B:668:MET:HE3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:NZ	1:B:552:GLU:OE2	2.40	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: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:A:668:MET:HE2	1:A:672:HIS:HB3	1.94	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:C:668:MET:HE2	1:C:672:HIS:HB3	1.94	0.49
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:B:337:LEU:HD23	1:B:668:MET:CE	2.42	0.49
1:C:595:ILE:HG13	1:C:615:TYR:CD2	2.48	0.49
1:C:255:GLY:HA3	1:C:686:ARG:CZ	2.43	0.49
1:B:105:TRP:HZ3	1:B:222:MET:HE1	1.78	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:337:LEU:HA	1:C:668:MET:HE3	1.97	0.45
1:C:110:GLU:OE1	1:C:110:GLU:N	2.34	0.45
1:B:33:GLU:HA	1:B:36:MET:HE3	1.97	0.45
1:D:388:ASP:HA	1:D:391:ASN:HB2	1.98	0.45
1:C:67:CYS:HG	1:C:84:CYS:HG	1.64	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: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:D:379:GLU:CD	1:D:531:ARG:HH22	2.20	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:A:32:ASN:HB3	1:A:36:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:HA	1:B:36:MET:CE	2.47	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: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:A:283:ILE:HA	1:A:287:THR:OG1	2.18	0.44
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
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: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: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: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: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:B:61:PRO:HB2	1:B:120:VAL:HG13	2.02	0.42
1:B:426:LYS:O	1:B:430:ILE:HG13	2.20	0.42
1:C:353:PHE:O	1:C:357:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:644:SER:OG	3:A:802:ASP:C	2.59	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:C:33:GLU:HA	1:C:36:MET:CE	2.50	0.41
1:A:28:LEU:HD22	1:A:36:MET:CE	2.50	0.41
1:A:32:ASN:HB3	1:A:36:MET:CE	2.50	0.41
1:A:358:ILE:HG13	1:A:359:ALA:N	2.36	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:C:105:TRP:HB3	1:C:107:MET:HE3	2.03	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:A:615:TYR:O	1:A:618:LYS:NZ	2.36	0.40
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:D:248:PHE:CZ	1:D:706:LYS:HE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:ASN:HB3	1:D:36:MET:HE2	2.02	0.40
1:D:433:GLN:HB3	1:D:436:PHE:CE2	2.56	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 (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	690/731 (94%)	647 (94%)	37 (5%)	6 (1%)	17	12
1	B	688/731 (94%)	662 (96%)	25 (4%)	1 (0%)	51	54
1	C	672/731 (92%)	641 (95%)	29 (4%)	2 (0%)	41	41
1	D	677/731 (93%)	633 (94%)	40 (6%)	4 (1%)	25	21
All	All	2727/2924 (93%)	2583 (95%)	131 (5%)	13 (0%)	29	26

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

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Mol	Chain	Res	Type
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 (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	577/631 (91%)	565 (98%)	12 (2%)	53	59
1	B	593/631 (94%)	590 (100%)	3 (0%)	88	92
1	C	538/631 (85%)	531 (99%)	7 (1%)	69	75
1	D	530/631 (84%)	525 (99%)	5 (1%)	78	84
All	All	2238/2524 (89%)	2211 (99%)	27 (1%)	71	77

All (27) 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	146	LYS
1	A	148	ASN
1	A	160	SER
1	A	271	THR
1	A	286	GLU
1	A	512	LYS
1	B	396	LYS
1	B	456	TYR
1	B	472	VAL
1	C	18	GLN

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Mol	Chain	Res	Type
1	C	46	ASP
1	C	229	LYS
1	C	271	THR
1	C	456	TYR
1	C	625	GLU
1	C	667	THR
1	D	73	SER
1	D	137	VAL
1	D	163	LYS
1	D	207	ASP
1	D	436	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	B	19	GLN
1	B	62	HIS
1	B	471	ASN
1	C	19	GLN
1	C	32	ASN
1	C	62	HIS
1	C	92	HIS
1	C	397	ASN
1	C	638	HIS
1	D	62	HIS

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 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	B	802	-	6,7,8	1.09	0	5,8,10	1.07	0
2	ARG	B	801	-	9,10,11	0.50	0	5,11,13	0.24	0
3	ASP	A	802	-	6,7,8	0.87	0	5,8,10	1.05	0
2	ARG	A	801	-	9,10,11	0.47	0	5,11,13	0.30	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	B	802	-	-	3/5/6/8	-
2	ARG	B	801	-	-	0/8/9/11	-
3	ASP	A	802	-	-	2/5/6/8	-
2	ARG	A	801	-	-	0/8/9/11	-

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 (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	694/731 (94%)	0.82	84 (12%) 4 5	35, 66, 106, 139	0
1	B	692/731 (94%)	0.41	21 (3%) 50 56	28, 50, 80, 99	0
1	C	682/731 (93%)	0.78	84 (12%) 4 5	28, 58, 108, 124	0
1	D	685/731 (93%)	1.12	133 (19%) 1 1	44, 73, 126, 143	0
All	All	2753/2924 (94%)	0.78	322 (11%) 4 6	28, 62, 112, 143	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	12.1
1	D	487	LEU	11.1
1	C	358	ILE	9.5
1	C	499	GLY	8.7
1	C	410	LEU	8.3
1	D	305	PHE	7.5
1	D	510	LEU	7.2
1	A	140	ILE	7.1
1	D	517	VAL	7.0
1	A	139	SER	6.8
1	D	522	ASP	6.6
1	D	422	PHE	6.6
1	D	493	PHE	6.5
1	A	138	ALA	6.3
1	D	491	ALA	6.2
1	D	413	VAL	6.2
1	C	491	ALA	6.2
1	D	137	VAL	6.1
1	A	501	ALA	5.8
1	D	297	ALA	5.8
1	D	477	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	17	LEU	5.7
1	D	311	ALA	5.7
1	D	316	TYR	5.7
1	D	479	PRO	5.7
1	A	16	THR	5.7
1	C	514	TYR	5.5
1	D	495	ALA	5.5
1	D	309	ASP	5.4
1	D	478	ALA	5.3
1	D	501	ALA	5.3
1	D	485	SER	5.3
1	D	410	LEU	5.3
1	D	476	LYS	5.2
1	C	360	ALA	5.1
1	D	308	LYS	5.1
1	D	486	LYS	5.1
1	D	165	ALA	5.0
1	D	497	LEU	5.0
1	D	131	ALA	5.0
1	D	508	ILE	4.9
1	D	474	TYR	4.9
1	D	504	VAL	4.8
1	D	458	THR	4.8
1	A	553	LEU	4.7
1	C	421	ALA	4.7
1	D	503	ALA	4.7
1	C	528	ILE	4.7
1	C	422	PHE	4.7
1	A	482	TYR	4.6
1	D	506	LYS	4.6
1	C	502	LYS	4.5
1	D	443	THR	4.5
1	D	304	GLY	4.5
1	D	461	PRO	4.5
1	C	411	GLU	4.5
1	D	449	PHE	4.5
1	D	480	SER	4.4
1	D	230	ASN	4.4
1	D	133	ILE	4.4
1	C	437	PHE	4.4
1	C	492	ASN	4.4
1	D	412	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	360	ALA	4.3
1	A	508	ILE	4.3
1	D	400	LEU	4.2
1	A	137	VAL	4.2
1	D	530	PRO	4.2
1	D	505	LEU	4.2
1	A	500	ASP	4.1
1	D	312	ILE	4.1
1	D	456	TYR	4.1
1	C	423	ASN	4.1
1	C	510	LEU	4.1
1	A	497	LEU	4.1
1	C	554	TYR	4.0
1	D	475	LYS	4.0
1	C	497	LEU	4.0
1	A	505	LEU	4.0
1	A	481	ILE	4.0
1	A	467	ILE	4.0
1	A	134	LEU	3.9
1	D	409	GLN	3.9
1	D	483	SER	3.9
1	A	473	GLU	3.8
1	D	439	ASP	3.8
1	A	136	GLY	3.8
1	C	508	ILE	3.8
1	D	16	THR	3.7
1	A	67	CYS	3.7
1	C	138	ALA	3.7
1	A	351	LYS	3.7
1	C	366	TYR	3.6
1	C	425	ARG	3.6
1	C	357	VAL	3.6
1	C	428	ASN	3.6
1	D	496	LEU	3.6
1	A	143	GLU	3.6
1	A	141	THR	3.6
1	A	144	THR	3.6
1	D	407	LEU	3.6
1	D	488	VAL	3.5
1	D	514	TYR	3.5
1	B	430	ILE	3.5
1	D	17	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	150	ILE	3.4
1	C	369	LEU	3.4
1	A	358	ILE	3.4
1	C	489	ASP	3.4
1	A	415	ILE	3.4
1	D	469	LEU	3.4
1	D	401	LEU	3.4
1	A	370	LEU	3.3
1	D	154	ILE	3.3
1	A	452	LEU	3.3
1	B	472	VAL	3.3
1	D	481	ILE	3.3
1	D	306	MET	3.3
1	D	498	SER	3.3
1	D	509	SER	3.3
1	A	449	PHE	3.2
1	D	423	ASN	3.2
1	A	642	GLY	3.2
1	C	414	PHE	3.2
1	B	165	ALA	3.2
1	D	645	GLY	3.2
1	A	567	LEU	3.2
1	A	640	THR	3.2
1	C	490	TYR	3.2
1	D	408	TYR	3.2
1	D	490	TYR	3.1
1	C	555	PRO	3.1
1	C	424	ASP	3.1
1	B	420	GLN	3.1
1	D	492	ASN	3.1
1	D	455	LEU	3.1
1	D	430	ILE	3.1
1	C	469	LEU	3.1
1	A	491	ALA	3.1
1	C	367	GLY	3.1
1	A	95	VAL	3.1
1	C	420	GLN	3.0
1	A	68	THR	3.0
1	C	362	LYS	3.0
1	A	361	GLY	3.0
1	B	483	SER	3.0
1	D	644	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	67	CYS	3.0
1	C	20	GLY	2.9
1	D	310	ASN	2.9
1	D	241	VAL	2.9
1	D	511	ASP	2.9
1	D	516	PHE	2.9
1	B	427	GLU	2.9
1	D	448	VAL	2.9
1	A	278	PHE	2.9
1	D	353	PHE	2.9
1	A	453	VAL	2.9
1	D	436	PHE	2.9
1	D	464	PHE	2.9
1	A	658	LEU	2.9
1	D	355	GLN	2.8
1	C	517	VAL	2.8
1	B	503	ALA	2.8
1	D	499	GLY	2.8
1	C	430	ILE	2.8
1	C	147	GLN	2.8
1	C	180	TYR	2.8
1	A	266	GLY	2.8
1	A	367	GLY	2.8
1	D	298	ALA	2.8
1	D	307	ARG	2.8
1	C	135	ASP	2.8
1	D	239	ASP	2.8
1	D	138	ALA	2.7
1	C	482	TYR	2.7
1	D	500	ASP	2.7
1	D	520	LEU	2.7
1	C	504	VAL	2.7
1	D	512	LYS	2.7
1	D	531	ARG	2.7
1	D	642	GLY	2.7
1	A	363	GLN	2.7
1	D	507	LYS	2.7
1	A	487	LEU	2.7
1	A	504	VAL	2.7
1	D	394	VAL	2.7
1	D	468	SER	2.7
1	D	403	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	314	ILE	2.7
1	D	549	ALA	2.7
1	C	498	SER	2.7
1	D	421	ALA	2.7
1	D	424	ASP	2.7
1	A	427	GLU	2.6
1	A	148	ASN	2.6
1	D	502	LYS	2.6
1	D	420	GLN	2.6
1	A	268	PRO	2.6
1	A	537	LEU	2.6
1	A	645	GLY	2.6
1	D	135	ASP	2.6
1	C	642	GLY	2.6
1	C	352	ASP	2.6
1	D	80	THR	2.6
1	A	643	ASN	2.6
1	C	354	GLN	2.6
1	D	553	LEU	2.6
1	A	639	THR	2.5
1	A	145	GLU	2.5
1	D	286	GLU	2.5
1	C	370	LEU	2.5
1	C	136	GLY	2.5
1	A	376	TYR	2.5
1	C	349	PHE	2.5
1	C	156	LYS	2.5
1	C	472	VAL	2.5
1	C	488	VAL	2.5
1	B	642	GLY	2.5
1	C	496	LEU	2.5
1	D	166	TRP	2.5
1	A	525	SER	2.5
1	C	495	ALA	2.5
1	C	553	LEU	2.5
1	D	157	VAL	2.5
1	A	84	CYS	2.4
1	C	449	PHE	2.4
1	C	309	ASP	2.4
1	B	141	THR	2.4
1	C	465	LEU	2.4
1	D	484	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	529	ALA	2.4
1	D	524	TYR	2.4
1	A	412	GLN	2.4
1	C	447	LYS	2.4
1	C	356	LYS	2.4
1	D	402	SER	2.4
1	D	447	LYS	2.4
1	D	451	GLN	2.4
1	A	267	TYR	2.4
1	A	264	VAL	2.3
1	C	532	TYR	2.3
1	D	376	TYR	2.3
1	D	405	TYR	2.3
1	A	369	LEU	2.3
1	A	465	LEU	2.3
1	D	442	SER	2.3
1	A	416	THR	2.3
1	C	427	GLU	2.3
1	D	145	GLU	2.3
1	C	685	MET	2.3
1	A	450	GLU	2.3
1	B	424	ASP	2.3
1	B	500	ASP	2.3
1	C	353	PHE	2.3
1	A	488	VAL	2.3
1	A	271	THR	2.3
1	A	135	ASP	2.3
1	C	527	ASN	2.3
1	A	147	GLN	2.3
1	B	474	TYR	2.3
1	D	79	LEU	2.3
1	D	627	GLY	2.3
1	D	296	GLU	2.3
1	A	239	ASP	2.2
1	A	353	PHE	2.2
1	C	493	PHE	2.2
1	D	144	THR	2.2
1	C	363	GLN	2.2
1	D	356	LYS	2.2
1	D	518	LYS	2.2
1	C	520	LEU	2.2
1	C	658	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	130	THR	2.2
1	A	366	TYR	2.2
1	D	389	TYR	2.2
1	D	411	GLU	2.2
1	A	21	GLY	2.2
1	A	69	SER	2.2
1	A	131	ALA	2.2
1	B	400	LEU	2.2
1	A	60	VAL	2.2
1	A	499	GLY	2.2
1	B	268	PRO	2.2
1	C	351	LYS	2.2
1	C	503	ALA	2.2
1	D	556	ASN	2.2
1	B	470	LEU	2.2
1	D	551	LEU	2.2
1	A	408	TYR	2.2
1	B	241	VAL	2.2
1	C	376	TYR	2.2
1	C	397	ASN	2.2
1	D	153	ASN	2.2
1	D	301	VAL	2.2
1	C	148	ASN	2.2
1	A	566	THR	2.2
1	C	68	THR	2.2
1	A	149	LYS	2.2
1	A	545	ILE	2.1
1	C	305	PHE	2.1
1	A	644	SER	2.1
1	A	466	PRO	2.1
1	C	408	TYR	2.1
1	C	537	LEU	2.1
1	D	129	VAL	2.1
1	D	446	GLU	2.1
1	A	265	MET	2.1
1	B	565	SER	2.1
1	D	229	LYS	2.1
1	C	18	GLN	2.1
1	D	646	SER	2.1
1	A	563	ALA	2.1
1	B	267	TYR	2.1
1	C	69	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	519	SER	2.0
1	D	519	SER	2.0
1	C	486	LYS	2.0
1	B	644	SER	2.0
1	B	68	THR	2.0
1	C	146	LYS	2.0
1	C	264	VAL	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
3	ASP	A	802	8/9	0.61	0.62	92,106,138,159	0
5	NA	D	803	1/1	0.86	0.10	57,57,57,57	0
2	ARG	A	801	11/12	0.90	0.23	60,69,82,82	0
4	CL	D	801	1/1	0.91	0.10	81,81,81,81	0
3	ASP	B	802	8/9	0.91	0.28	35,44,61,68	8
2	ARG	B	801	11/12	0.94	0.19	33,44,57,60	0
4	CL	C	801	1/1	0.95	0.17	53,53,53,53	0
4	CL	D	802	1/1	0.98	0.23	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.