Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 11:53 am BST

PDB ID	:	5JRL
Title	:	Crystal Structure of the Sphingopyxin I Lasso Peptide Isopeptidase SpI-IsoP (Native)
Authors	:	Fage, C.D.; Hegemann, J.D.; Bange, G.; Marahiel, M.A.
Deposited on	:	2016-05-06
Resolution	:	3.20 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11
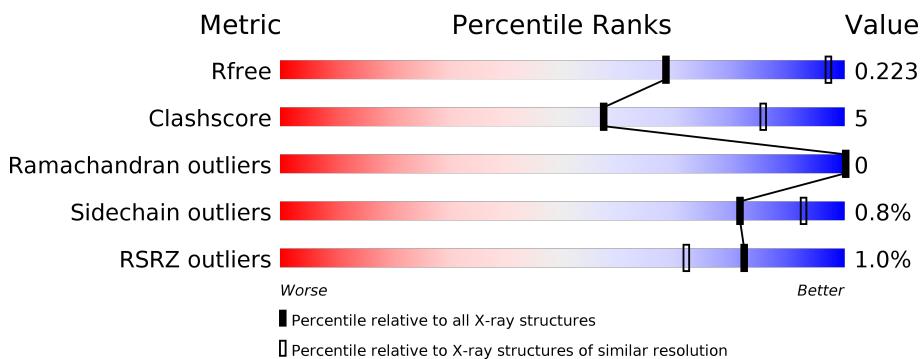
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
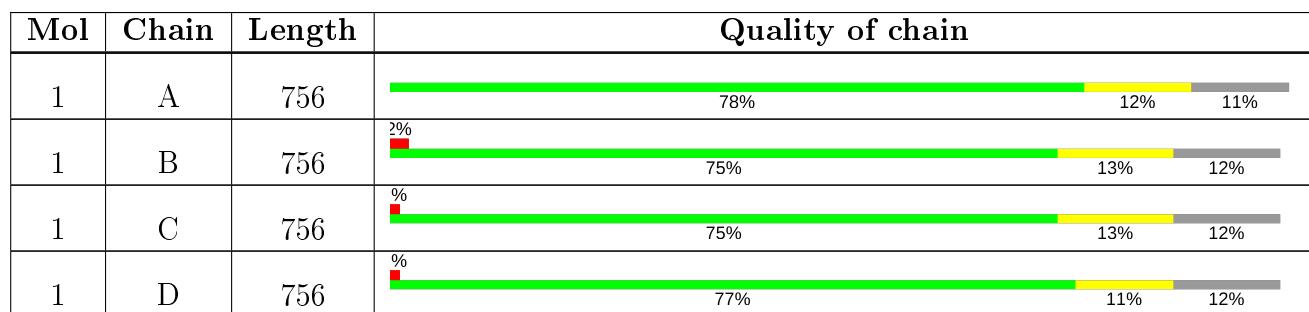
The reported resolution of this entry is 3.20 Å.

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	Percentile Ranks	Value
Rfree		0.223
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		1.0%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	756	78% 12% 11%
1	B	756	2% 75% 13% 12%
1	C	756	% 75% 13% 12%
1	D	756	% 77% 11% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20892 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 Dipeptidyl aminopeptidases/acylaminoacyl-peptidases-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total 5265	C 3297	N 964	O 991	S 13	0	0	0
1	B	666	Total 5210	C 3264	N 952	O 980	S 14	0	0	0
1	C	664	Total 5192	C 3258	N 946	O 976	S 12	0	0	0
1	D	669	Total 5225	C 3274	N 957	O 981	S 13	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1GQ33
A	-18	GLY	-	expression tag	UNP Q1GQ33
A	-17	SER	-	expression tag	UNP Q1GQ33
A	-16	SER	-	expression tag	UNP Q1GQ33
A	-15	HIS	-	expression tag	UNP Q1GQ33
A	-14	HIS	-	expression tag	UNP Q1GQ33
A	-13	HIS	-	expression tag	UNP Q1GQ33
A	-12	HIS	-	expression tag	UNP Q1GQ33
A	-11	HIS	-	expression tag	UNP Q1GQ33
A	-10	HIS	-	expression tag	UNP Q1GQ33
A	-9	SER	-	expression tag	UNP Q1GQ33
A	-8	SER	-	expression tag	UNP Q1GQ33
A	-7	GLY	-	expression tag	UNP Q1GQ33
A	-6	LEU	-	expression tag	UNP Q1GQ33
A	-5	VAL	-	expression tag	UNP Q1GQ33
A	-4	PRO	-	expression tag	UNP Q1GQ33
A	-3	ARG	-	expression tag	UNP Q1GQ33
A	-2	GLY	-	expression tag	UNP Q1GQ33
A	-1	SER	-	expression tag	UNP Q1GQ33
A	0	HIS	-	expression tag	UNP Q1GQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	727	SER	-	expression tag	UNP Q1GQ33
A	728	ALA	-	expression tag	UNP Q1GQ33
A	729	TRP	-	expression tag	UNP Q1GQ33
A	730	SER	-	expression tag	UNP Q1GQ33
A	731	HIS	-	expression tag	UNP Q1GQ33
A	732	PRO	-	expression tag	UNP Q1GQ33
A	733	GLN	-	expression tag	UNP Q1GQ33
A	734	PHE	-	expression tag	UNP Q1GQ33
A	735	GLU	-	expression tag	UNP Q1GQ33
A	736	LYS	-	expression tag	UNP Q1GQ33
B	-19	MET	-	initiating methionine	UNP Q1GQ33
B	-18	GLY	-	expression tag	UNP Q1GQ33
B	-17	SER	-	expression tag	UNP Q1GQ33
B	-16	SER	-	expression tag	UNP Q1GQ33
B	-15	HIS	-	expression tag	UNP Q1GQ33
B	-14	HIS	-	expression tag	UNP Q1GQ33
B	-13	HIS	-	expression tag	UNP Q1GQ33
B	-12	HIS	-	expression tag	UNP Q1GQ33
B	-11	HIS	-	expression tag	UNP Q1GQ33
B	-10	HIS	-	expression tag	UNP Q1GQ33
B	-9	SER	-	expression tag	UNP Q1GQ33
B	-8	SER	-	expression tag	UNP Q1GQ33
B	-7	GLY	-	expression tag	UNP Q1GQ33
B	-6	LEU	-	expression tag	UNP Q1GQ33
B	-5	VAL	-	expression tag	UNP Q1GQ33
B	-4	PRO	-	expression tag	UNP Q1GQ33
B	-3	ARG	-	expression tag	UNP Q1GQ33
B	-2	GLY	-	expression tag	UNP Q1GQ33
B	-1	SER	-	expression tag	UNP Q1GQ33
B	0	HIS	-	expression tag	UNP Q1GQ33
B	727	SER	-	expression tag	UNP Q1GQ33
B	728	ALA	-	expression tag	UNP Q1GQ33
B	729	TRP	-	expression tag	UNP Q1GQ33
B	730	SER	-	expression tag	UNP Q1GQ33
B	731	HIS	-	expression tag	UNP Q1GQ33
B	732	PRO	-	expression tag	UNP Q1GQ33
B	733	GLN	-	expression tag	UNP Q1GQ33
B	734	PHE	-	expression tag	UNP Q1GQ33
B	735	GLU	-	expression tag	UNP Q1GQ33
B	736	LYS	-	expression tag	UNP Q1GQ33
C	-19	MET	-	initiating methionine	UNP Q1GQ33
C	-18	GLY	-	expression tag	UNP Q1GQ33

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| Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP Q1GQ33
C	-16	SER	-	expression tag	UNP Q1GQ33
C	-15	HIS	-	expression tag	UNP Q1GQ33
C	-14	HIS	-	expression tag	UNP Q1GQ33
C	-13	HIS	-	expression tag	UNP Q1GQ33
C	-12	HIS	-	expression tag	UNP Q1GQ33
C	-11	HIS	-	expression tag	UNP Q1GQ33
C	-10	HIS	-	expression tag	UNP Q1GQ33
C	-9	SER	-	expression tag	UNP Q1GQ33
C	-8	SER	-	expression tag	UNP Q1GQ33
C	-7	GLY	-	expression tag	UNP Q1GQ33
C	-6	LEU	-	expression tag	UNP Q1GQ33
C	-5	VAL	-	expression tag	UNP Q1GQ33
C	-4	PRO	-	expression tag	UNP Q1GQ33
C	-3	ARG	-	expression tag	UNP Q1GQ33
C	-2	GLY	-	expression tag	UNP Q1GQ33
C	-1	SER	-	expression tag	UNP Q1GQ33
C	0	HIS	-	expression tag	UNP Q1GQ33
C	727	SER	-	expression tag	UNP Q1GQ33
C	728	ALA	-	expression tag	UNP Q1GQ33
C	729	TRP	-	expression tag	UNP Q1GQ33
C	730	SER	-	expression tag	UNP Q1GQ33
C	731	HIS	-	expression tag	UNP Q1GQ33
C	732	PRO	-	expression tag	UNP Q1GQ33
C	733	GLN	-	expression tag	UNP Q1GQ33
C	734	PHE	-	expression tag	UNP Q1GQ33
C	735	GLU	-	expression tag	UNP Q1GQ33
C	736	LYS	-	expression tag	UNP Q1GQ33
D	-19	MET	-	initiating methionine	UNP Q1GQ33
D	-18	GLY	-	expression tag	UNP Q1GQ33
D	-17	SER	-	expression tag	UNP Q1GQ33
D	-16	SER	-	expression tag	UNP Q1GQ33
D	-15	HIS	-	expression tag	UNP Q1GQ33
D	-14	HIS	-	expression tag	UNP Q1GQ33
D	-13	HIS	-	expression tag	UNP Q1GQ33
D	-12	HIS	-	expression tag	UNP Q1GQ33
D	-11	HIS	-	expression tag	UNP Q1GQ33
D	-10	HIS	-	expression tag	UNP Q1GQ33
D	-9	SER	-	expression tag	UNP Q1GQ33
D	-8	SER	-	expression tag	UNP Q1GQ33
D	-7	GLY	-	expression tag	UNP Q1GQ33
D	-6	LEU	-	expression tag	UNP Q1GQ33

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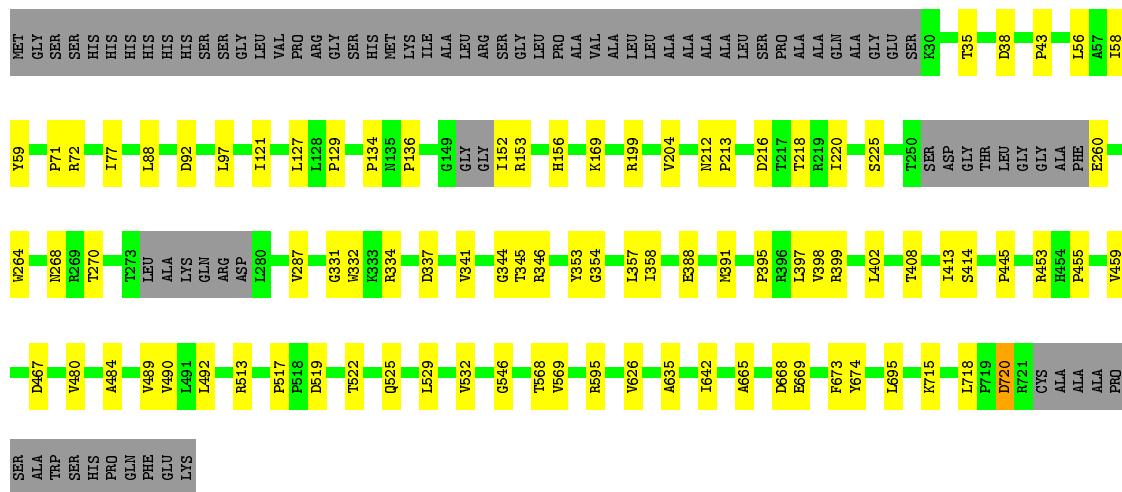
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	expression tag	UNP Q1GQ33
D	-4	PRO	-	expression tag	UNP Q1GQ33
D	-3	ARG	-	expression tag	UNP Q1GQ33
D	-2	GLY	-	expression tag	UNP Q1GQ33
D	-1	SER	-	expression tag	UNP Q1GQ33
D	0	HIS	-	expression tag	UNP Q1GQ33
D	727	SER	-	expression tag	UNP Q1GQ33
D	728	ALA	-	expression tag	UNP Q1GQ33
D	729	TRP	-	expression tag	UNP Q1GQ33
D	730	SER	-	expression tag	UNP Q1GQ33
D	731	HIS	-	expression tag	UNP Q1GQ33
D	732	PRO	-	expression tag	UNP Q1GQ33
D	733	GLN	-	expression tag	UNP Q1GQ33
D	734	PHE	-	expression tag	UNP Q1GQ33
D	735	GLU	-	expression tag	UNP Q1GQ33
D	736	LYS	-	expression tag	UNP Q1GQ33

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
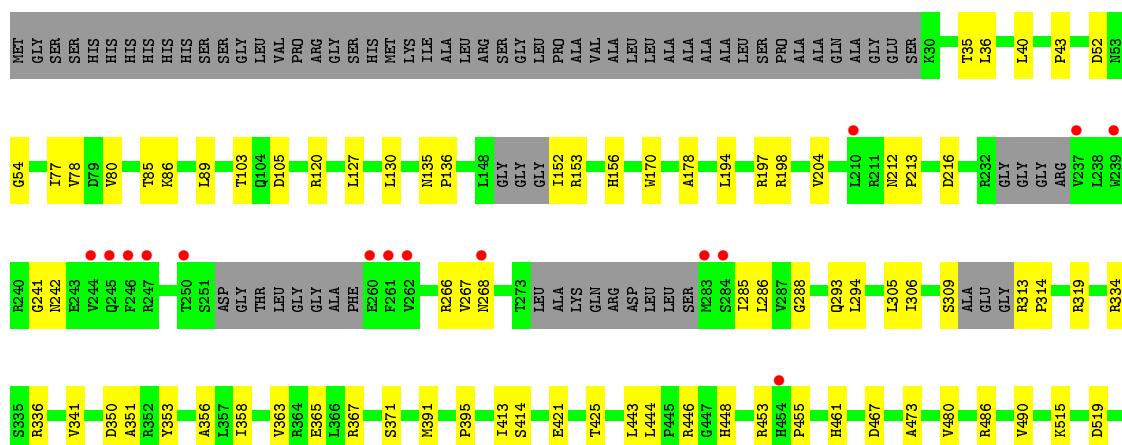
• Molecule 1: Dipeptidyl aminopeptidases/acylaminoacyl-peptidases-like protein
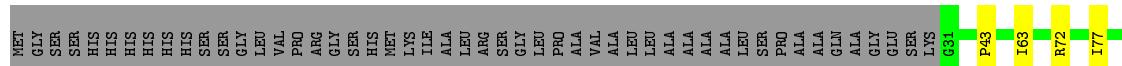
• Molecule 1: Dipeptidyl aminopeptidases/acylaminoacyl-peptidases-like protein

• Molecule 1: Dipeptidyl aminopeptidases/acylaminoacyl-peptidases-like protein

Chain C:

• Molecule 1: Dipeptidyl aminopeptidases/acylaminoacyl-peptidases-like protein

Chain D:
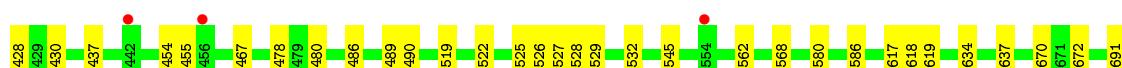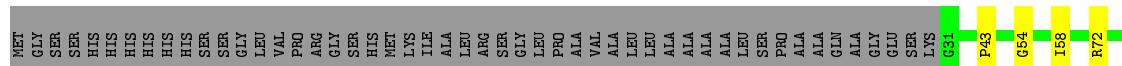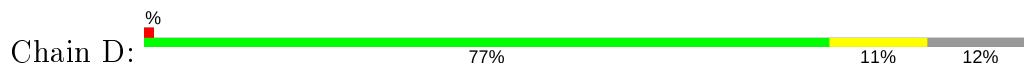
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.47Å 136.59Å 110.78Å 90.00° 97.62° 90.00°	Depositor
Resolution (Å)	48.39 – 3.20 48.39 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.39-3.20) 99.7 (48.39-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10-2152	Depositor
R, R_{free}	0.221 , 0.266 0.223 , 0.223	Depositor DCC
R_{free} test set	2572 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	81.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20892	wwPDB-VP
Average B, all atoms (Å^2)	79.0	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.24	0/5379	0.44	0/7303
1	B	0.24	0/5322	0.44	0/7225
1	C	0.24	0/5305	0.44	0/7204
1	D	0.28	1/5339 (0.0%)	0.44	0/7250
All	All	0.25	1/21345 (0.0%)	0.44	0/28982

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	TYR	C-N	10.10	1.53	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5265	0	5197	53	0
1	B	5210	0	5137	58	0
1	C	5192	0	5118	56	0
1	D	5225	0	5144	44	0
All	All	20892	0	20596	204	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 (204) 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:D:400:VAL:HG22	1:D:407:ILE:HG22	1.67	0.75
1:B:309:SER:HG	1:B:313:ARG:N	1.89	0.70
1:B:170:TRP:HE1	1:B:213:PRO:HD3	1.57	0.69
1:B:480:VAL:HG13	1:B:490:VAL:HG11	1.75	0.68
1:B:395:PRO:HB2	1:B:413:ILE:HD12	1.77	0.67
1:C:400:VAL:HG22	1:C:407:ILE:HG22	1.77	0.67
1:B:306:ILE:HD11	1:B:314:PRO:HB2	1.81	0.62
1:B:525:GLN:HA	1:B:529:LEU:HB2	1.80	0.62
1:B:212:ASN:HD21	1:B:216:ASP:HB2	1.65	0.62
1:B:152:ILE:HG13	1:B:153:ARG:H	1.66	0.60
1:D:299:LEU:O	1:D:303:ARG:NH1	2.35	0.60
1:B:453:ARG:HE	1:B:546:GLY:HA2	1.67	0.59
1:D:178:ALA:HA	1:D:204:VAL:HG12	1.84	0.59
1:B:288:GLY:O	1:B:334:ARG:NH1	2.33	0.59
1:A:199:ARG:NH1	1:A:668:ASP:OD1	2.34	0.59
1:C:453:ARG:HE	1:C:546:GLY:HA2	1.67	0.59
1:C:212:ASN:HD21	1:C:216:ASP:HB2	1.68	0.59
1:A:480:VAL:HG13	1:A:490:VAL:HG11	1.85	0.58
1:C:152:ILE:HG13	1:C:153:ARG:H	1.68	0.58
1:D:152:ILE:HG13	1:D:153:ARG:H	1.69	0.58
1:D:169:LYS:HB3	1:D:213:PRO:HG3	1.86	0.58
1:A:152:ILE:HG13	1:A:153:ARG:H	1.69	0.58
1:B:461:HIS:ND1	1:B:473:ALA:O	2.31	0.58
1:B:455:PRO:HG3	1:B:695:LEU:HD21	1.86	0.58
1:C:199:ARG:NH1	1:C:668:ASP:OD1	2.37	0.58
1:A:199:ARG:NH2	1:A:665:ALA:O	2.38	0.57
1:B:305:LEU:HD23	1:B:363:VAL:HG21	1.86	0.57
1:B:103:THR:HG22	1:B:105:ASP:H	1.70	0.57
1:C:519:ASP:HB3	1:C:522:THR:HG23	1.86	0.57
1:C:525:GLN:HA	1:C:529:LEU:HB2	1.86	0.57
1:C:169:LYS:HB3	1:C:213:PRO:HG3	1.87	0.56
1:D:177:ARG:NH2	1:D:205:GLU:OE1	2.38	0.56
1:A:715:LYS:HA	1:A:718:LEU:HD13	1.87	0.56
1:C:587:GLU:OE1	1:C:620:SER:OG	2.20	0.56
1:D:525:GLN:HA	1:D:529:LEU:HB2	1.87	0.56
1:B:319:ARG:H	1:C:273:THR:HG23	1.69	0.56
1:B:486:ARG:NH2	1:B:691:ASP:OD2	2.34	0.55
1:C:395:PRO:HB2	1:C:413:ILE:HD12	1.88	0.55
1:D:519:ASP:HB2	1:D:522:THR:HG23	1.88	0.55
1:D:322:PHE:HA	1:D:347:GLY:HA2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ARG:NH2	1:A:517:PRO:O	2.40	0.55
1:B:120:ARG:HB2	1:B:130:LEU:HD12	1.87	0.55
1:A:334:ARG:HG3	1:A:341:VAL:HG12	1.88	0.54
1:C:178:ALA:HA	1:C:204:VAL:HG12	1.89	0.54
1:C:425:THR:HG22	1:C:443:LEU:HD13	1.90	0.54
1:C:194:LEU:HB3	1:C:197:ARG:HD3	1.90	0.54
1:D:398:VAL:HG12	1:D:409:ASP:HA	1.90	0.54
1:C:139:VAL:HG22	1:C:140:GLY:H	1.73	0.53
1:B:89:LEU:HD23	1:B:127:LEU:HD21	1.91	0.53
1:B:241:GLY:O	1:B:266:ARG:NH1	2.42	0.53
1:D:58:ILE:HG13	1:D:97:LEU:HD21	1.91	0.53
1:B:294:LEU:HD12	1:B:305:LEU:HD11	1.91	0.53
1:D:391:MET:N	1:D:467:ASP:OD1	2.42	0.52
1:D:480:VAL:HG13	1:D:490:VAL:HG11	1.90	0.52
1:A:346:ARG:NH1	1:A:353:TYR:OH	2.41	0.52
1:B:341:VAL:HG23	1:B:358:ILE:HB	1.91	0.51
1:B:391:MET:N	1:B:467:ASP:OD1	2.43	0.51
1:A:519:ASP:HB3	1:A:522:THR:HG23	1.92	0.51
1:C:357:LEU:HD11	1:C:402:LEU:HD22	1.92	0.51
1:A:169:LYS:HB3	1:A:213:PRO:HG3	1.92	0.51
1:C:532:VAL:HG13	1:C:568:THR:HG22	1.91	0.51
1:D:304:GLU:OE1	1:D:319:ARG:NH1	2.44	0.51
1:C:322:PHE:HA	1:C:347:GLY:HA2	1.91	0.51
1:C:288:GLY:O	1:C:334:ARG:NH1	2.44	0.51
1:C:391:MET:N	1:C:467:ASP:OD1	2.44	0.51
1:C:177:ARG:NH2	1:C:205:GLU:OE1	2.45	0.51
1:B:334:ARG:HA	1:B:341:VAL:HG12	1.93	0.50
1:D:532:VAL:HG13	1:D:568:THR:HG22	1.94	0.50
1:D:58:ILE:HD11	1:D:97:LEU:HD11	1.92	0.50
1:D:395:PRO:HB2	1:D:413:ILE:HD12	1.94	0.50
1:C:704:PHE:HB2	1:C:707:HIS:CD2	2.47	0.49
1:B:608:SER:O	1:B:611:ILE:HG13	2.13	0.49
1:A:455:PRO:HG3	1:A:695:LEU:HD21	1.95	0.49
1:A:72:ARG:NH1	1:A:92:ASP:OD1	2.46	0.49
1:B:350:ASP:OD2	1:B:367:ARG:NH2	2.46	0.49
1:C:707:HIS:O	1:C:710:LYS:N	2.46	0.49
1:B:421:GLU:OE2	1:B:446:ARG:NH2	2.46	0.49
1:A:212:ASN:HD21	1:A:216:ASP:HB2	1.77	0.48
1:A:341:VAL:HG22	1:A:358:ILE:HB	1.95	0.48
1:A:56:LEU:HD23	1:A:77:ILE:HD11	1.93	0.48
1:D:428:ARG:NH2	1:D:545:GLU:OE2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PRO:HG3	1:A:414:SER:HB2	1.96	0.48
1:B:178:ALA:HA	1:B:204:VAL:HG12	1.93	0.48
1:D:486:ARG:NH1	1:D:691:ASP:OD2	2.46	0.48
1:B:43:PRO:HG3	1:B:414:SER:HB2	1.96	0.48
1:C:396:ARG:HG3	1:C:412:PRO:HA	1.94	0.48
1:A:357:LEU:HD11	1:A:402:LEU:HD22	1.95	0.48
1:A:445:PRO:HD3	1:A:489:VAL:HG22	1.96	0.48
1:A:204:VAL:O	1:A:225:SER:OG	2.29	0.48
1:A:445:PRO:HA	1:A:484:ALA:HB1	1.95	0.48
1:B:309:SER:OG	1:B:313:ARG:N	2.45	0.48
1:A:287:VAL:HG12	1:A:332:TRP:CZ2	2.49	0.47
1:A:532:VAL:HG13	1:A:568:THR:HG22	1.96	0.47
1:B:242:ASN:HA	1:B:266:ARG:NH2	2.29	0.47
1:C:304:GLU:HG2	1:C:319:ARG:HD3	1.95	0.47
1:A:399:ARG:HH21	1:A:408:THR:HG21	1.79	0.47
1:C:475:GLN:OE1	1:C:481:GLN:NE2	2.36	0.47
1:C:77:ILE:HB	1:C:88:LEU:HD11	1.94	0.47
1:B:425:THR:HG22	1:B:443:LEU:HD13	1.95	0.47
1:A:331:GLY:O	1:A:344:GLY:N	2.39	0.47
1:C:670:THR:OG1	1:C:672:VAL:O	2.27	0.47
1:D:194:LEU:HB3	1:D:197:ARG:HD3	1.97	0.47
1:D:454:HIS:HB2	1:D:489:VAL:HG23	1.96	0.47
1:A:642:ILE:HG23	1:C:192:THR:HG22	1.97	0.46
1:C:43:PRO:HG3	1:C:414:SER:HB2	1.96	0.46
1:C:361:THR:OG1	1:C:362:GLY:N	2.48	0.46
1:D:43:PRO:HG3	1:D:414:SER:HB2	1.97	0.46
1:D:562:SER:OG	1:D:580:SER:OG	2.19	0.46
1:A:58:ILE:HG23	1:A:97:LEU:HD21	1.98	0.46
1:B:52:ASP:OD1	1:B:336:ARG:NH2	2.48	0.46
1:B:367:ARG:NH1	1:C:268:ASN:O	2.48	0.46
1:B:558:TYR:HA	1:B:562:SER:HB3	1.97	0.46
1:D:72:ARG:HH21	1:D:90:THR:HG23	1.79	0.46
1:B:170:TRP:NE1	1:B:213:PRO:HD3	2.28	0.46
1:A:459:VAL:HB	1:A:492:LEU:HD23	1.97	0.46
1:D:152:ILE:HD12	1:D:152:ILE:HA	1.86	0.46
1:B:670:THR:OG1	1:B:672:VAL:O	2.27	0.45
1:A:525:GLN:HA	1:A:529:LEU:HB2	1.98	0.45
1:B:266:ARG:HB2	1:B:266:ARG:HE	1.53	0.45
1:B:35:THR:HG22	1:B:36:LEU:N	2.32	0.45
1:A:453:ARG:HE	1:A:546:GLY:HA2	1.82	0.45
1:A:395:PRO:HB2	1:A:413:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:PRO:HG3	1:D:695:LEU:HD21	1.99	0.45
1:D:699:ASP:HB2	1:D:702:ALA:HB2	1.99	0.44
1:C:559:SER:HB2	1:C:671:HIS:NE2	2.32	0.44
1:D:204:VAL:O	1:D:225:SER:OG	2.36	0.44
1:A:635:ALA:HB2	1:A:673:PHE:HE1	1.82	0.44
1:B:194:LEU:HB3	1:B:197:ARG:HD3	1.99	0.44
1:C:352:ARG:HG3	1:C:371:SER:HB3	2.00	0.44
1:B:519:ASP:HB2	1:B:522:THR:HG23	2.00	0.44
1:B:353:TYR:HD2	1:B:371:SER:HG	1.66	0.43
1:A:268:ASN:HB3	1:A:270:THR:HG23	2.00	0.43
1:A:77:ILE:HB	1:A:88:LEU:HD11	1.99	0.43
1:C:367:ARG:HA	1:C:367:ARG:HD3	1.87	0.43
1:C:669:GLU:OE1	1:C:673:PHE:HA	2.18	0.43
1:B:136:PRO:HB2	1:B:156:HIS:HB3	2.01	0.43
1:C:664:THR:HG22	1:C:665:ALA:N	2.33	0.43
1:B:707:HIS:O	1:B:710:LYS:N	2.52	0.43
1:C:208:PHE:O	1:C:220:ILE:N	2.47	0.43
1:B:358:ILE:HG23	1:B:363:VAL:HG22	2.01	0.43
1:B:54:GLY:O	1:B:80:VAL:HG21	2.19	0.43
1:C:357:LEU:HD21	1:C:402:LEU:HB3	2.00	0.43
1:A:595:ARG:NH2	1:C:646:GLU:OE1	2.52	0.43
1:D:527:LEU:HB2	1:D:528:TRP:CE3	2.54	0.43
1:A:71:PRO:HD3	1:A:674:TYR:O	2.19	0.43
1:A:35:THR:OG1	1:A:38:ASP:OD1	2.37	0.43
1:C:334:ARG:HG3	1:C:341:VAL:HG12	2.01	0.43
1:C:510:ALA:HB2	1:C:518:PRO:HD2	2.01	0.43
1:D:335:SER:HA	1:D:381:LEU:HD13	2.01	0.43
1:A:260:GLU:N	1:A:260:GLU:OE1	2.52	0.42
1:A:136:PRO:HB2	1:A:156:HIS:HB3	2.01	0.42
1:A:720:ASP:N	1:A:720:ASP:OD1	2.51	0.42
1:B:444:LEU:HD13	1:B:448:HIS:CD2	2.54	0.42
1:B:532:VAL:HB	1:B:568:THR:HG22	2.01	0.42
1:B:77:ILE:HG22	1:B:86:LYS:HB3	2.01	0.42
1:B:78:VAL:HG22	1:B:85:THR:HG22	2.00	0.42
1:C:515:LYS:HE3	1:C:515:LYS:HB2	1.81	0.42
1:C:438:SER:HG	1:C:534:SER:HG	1.67	0.42
1:C:682:ALA:O	1:C:686:ASN:ND2	2.52	0.42
1:D:526:LYS:HA	1:D:526:LYS:HD3	1.86	0.42
1:A:121:ILE:HG12	1:A:127:LEU:HB3	2.01	0.42
1:B:562:SER:HB2	1:B:580:SER:OG	2.20	0.42
1:D:357:LEU:HD21	1:D:402:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:HG23	1:A:264:TRP:CE3	2.55	0.42
1:B:564:MET:O	1:B:568:THR:HG23	2.19	0.42
1:B:198:ARG:NH2	1:B:639:PRO:HD3	2.34	0.42
1:C:43:PRO:HB3	1:C:63:ILE:HG12	2.02	0.42
1:D:268:ASN:HB3	1:D:270:THR:HG23	2.00	0.42
1:B:356:ALA:HA	1:B:365:GLU:HA	2.01	0.42
1:D:430:PHE:O	1:D:437:TRP:HA	2.20	0.42
1:D:78:VAL:HG22	1:D:85:THR:HG22	2.01	0.41
1:A:129:PRO:HB2	1:D:134:PRO:HB2	2.02	0.41
1:B:267:VAL:HG23	1:B:268:ASN:H	1.85	0.41
1:A:218:THR:HA	1:D:216:ASP:HB2	2.01	0.41
1:A:569:VAL:HG12	1:A:626:VAL:HG22	2.03	0.41
1:B:350:ASP:OD1	1:B:351:ALA:N	2.53	0.41
1:D:54:GLY:O	1:D:80:VAL:HG21	2.20	0.41
1:B:40:LEU:HD22	1:B:680:LEU:HD21	2.02	0.41
1:C:443:LEU:HB3	1:C:490:VAL:HG13	2.01	0.41
1:C:568:THR:O	1:C:572:SER:N	2.53	0.41
1:D:634:VAL:CG1	1:D:637:ALA:H	2.34	0.41
1:A:59:TYR:CE1	1:A:397:LEU:HD11	2.55	0.41
1:B:152:ILE:HA	1:B:152:ILE:HD12	1.87	0.41
1:C:139:VAL:HG12	1:C:155:SER:O	2.21	0.41
1:A:345:THR:HG22	1:A:354:GLY:C	2.40	0.41
1:A:391:MET:N	1:A:467:ASP:OD1	2.54	0.41
1:A:532:VAL:HG22	1:A:568:THR:HG22	2.03	0.41
1:C:170:TRP:CZ2	1:C:266:ARG:HD3	2.55	0.41
1:A:287:VAL:HG12	1:A:332:TRP:HZ2	1.84	0.41
1:C:152:ILE:HA	1:C:152:ILE:HD12	1.86	0.41
1:D:334:ARG:HG3	1:D:341:VAL:HG12	2.02	0.41
1:D:586:LEU:HD22	1:D:617:PHE:HE2	1.86	0.41
1:D:670:THR:OG1	1:D:672:VAL:O	2.26	0.41
1:C:72:ARG:NH1	1:C:92:ASP:OD1	2.54	0.41
1:A:134:PRO:HB2	1:D:129:PRO:HB2	2.03	0.41
1:A:152:ILE:HA	1:A:152:ILE:HD12	1.88	0.40
1:C:634:VAL:CG1	1:C:637:ALA:H	2.34	0.40
1:A:388:GLU:OE1	1:A:398:VAL:HG11	2.22	0.40
1:B:285:ILE:CG2	1:B:286:LEU:N	2.85	0.40
1:C:335:SER:HA	1:C:381:LEU:HD13	2.03	0.40
1:C:199:ARG:NH2	1:C:665:ALA:O	2.54	0.40
1:A:220:ILE:HG23	1:A:264:TRP:CD2	2.57	0.40
1:C:346:ARG:NH1	1:C:353:TYR:OH	2.55	0.40
1:D:618:ALA:HA	1:D:619:PRO:HD3	1.95	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	667/756 (88%)	647 (97%)	20 (3%)	0	100	100
1	B	654/756 (86%)	634 (97%)	20 (3%)	0	100	100
1	C	652/756 (86%)	625 (96%)	27 (4%)	0	100	100
1	D	659/756 (87%)	640 (97%)	19 (3%)	0	100	100
All	All	2632/3024 (87%)	2546 (97%)	86 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	555/610 (91%)	552 (100%)	3 (0%)	88	95
1	B	552/610 (90%)	549 (100%)	3 (0%)	88	95
1	C	548/610 (90%)	545 (100%)	3 (0%)	88	95
1	D	550/610 (90%)	542 (98%)	8 (2%)	65	85
All	All	2205/2440 (90%)	2188 (99%)	17 (1%)	81	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	ASP
1	A	669	GLU
1	A	720	ASP
1	B	135	ASN
1	B	293	GLN
1	B	515	LYS
1	C	135	ASN
1	C	195	LEU
1	C	669	GLU
1	D	135	ASN
1	D	228	ARG
1	D	274	LEU
1	D	293	GLN
1	D	303	ARG
1	D	315	HIS
1	D	701	ASP
1	D	706	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	675/756 (89%)	-0.23	0	100	100	32, 65, 100, 128	0
1	B	666/756 (88%)	0.05	15 (2%)	60	47	47, 87, 121, 142	0
1	C	664/756 (87%)	-0.10	5 (0%)	86	78	48, 77, 113, 128	0
1	D	669/756 (88%)	0.01	6 (0%)	84	75	40, 81, 116, 133	0
All	All	2674/3024 (88%)	-0.07	26 (0%)	82	72	32, 77, 115, 142	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	GLY	5.3
1	B	283	MET	4.4
1	B	245	GLN	3.9
1	D	287	VAL	3.3
1	B	268	ASN	3.3
1	B	250	THR	3.1
1	D	456	ALA	3.0
1	B	262	VAL	2.8
1	C	308	THR	2.8
1	B	246	PHE	2.8
1	B	261	PHE	2.7
1	C	356	ALA	2.7
1	B	454	HIS	2.7
1	B	247	ARG	2.7
1	B	237	VAL	2.7
1	B	239	TRP	2.6
1	B	210	LEU	2.6
1	C	720	ASP	2.6
1	D	442	VAL	2.5
1	D	402	LEU	2.3
1	B	260	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	284	SER	2.1
1	D	554	GLY	2.1
1	C	444	LEU	2.1
1	B	244	VAL	2.1
1	C	294	LEU	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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.