



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:43 PM UTC

PDB ID : 5JRK / pdb_00005jrk
Title : Crystal Structure of the Sphingopyxin I Lasso Peptide Isopeptidase SpI-IsoP
(SeMet-derived)
Authors : Fage, C.D.; Hegemann, J.D.; Bange, G.; Marahiel, M.A.
Deposited on : 2016-05-06
Resolution : 3.00 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

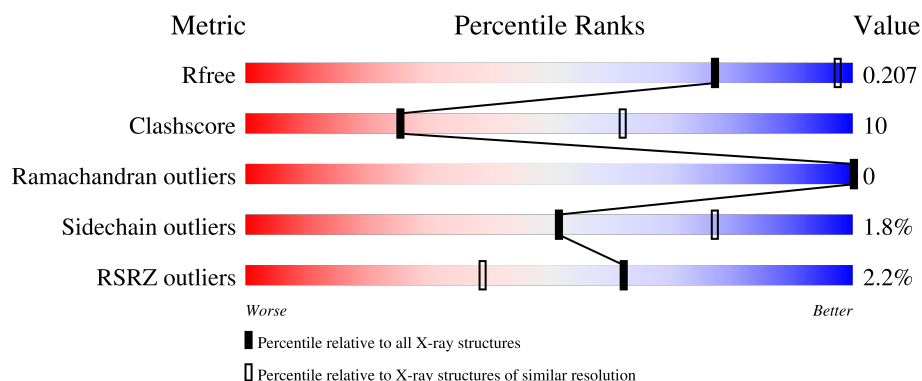
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	756	70% 21% 8%
1	B	756	3% 68% 21% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10681 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	695	Total	C	N	O	S	Se	0	0	0
			5393	3373	989	1017	4	10			
1	B	677	Total	C	N	O	S	Se	0	0	0
			5264	3295	967	989	4	9			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	MSE	-	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

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).

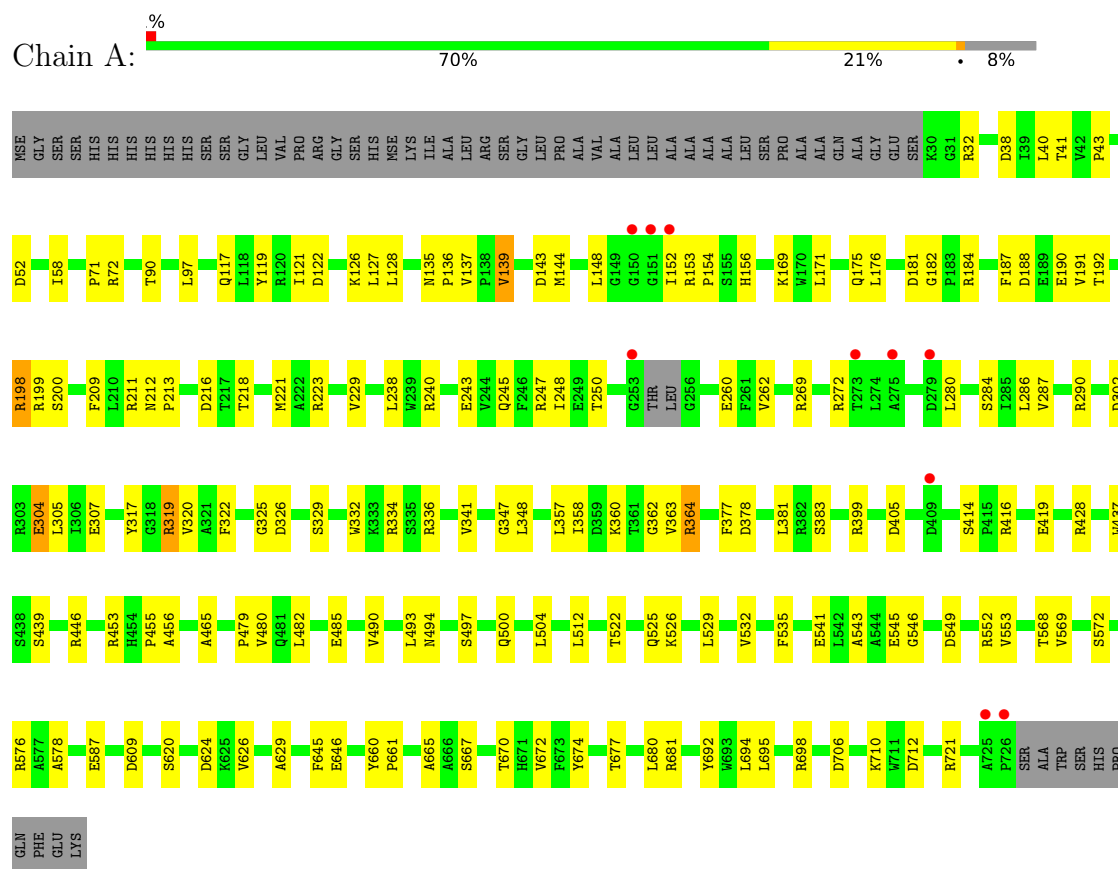


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

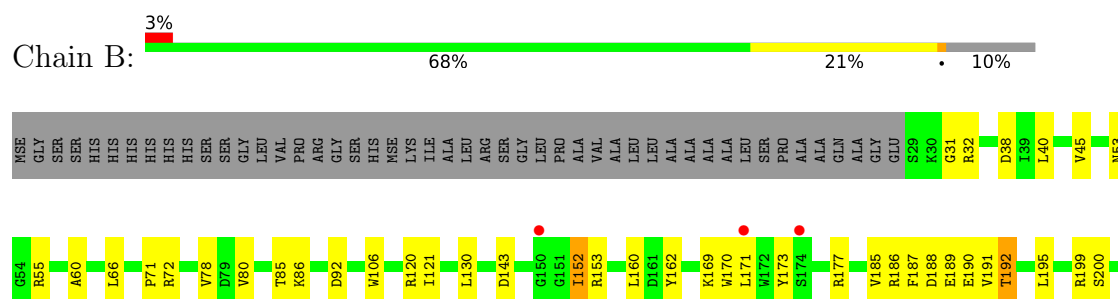
3 Residue-property plots [i](#)

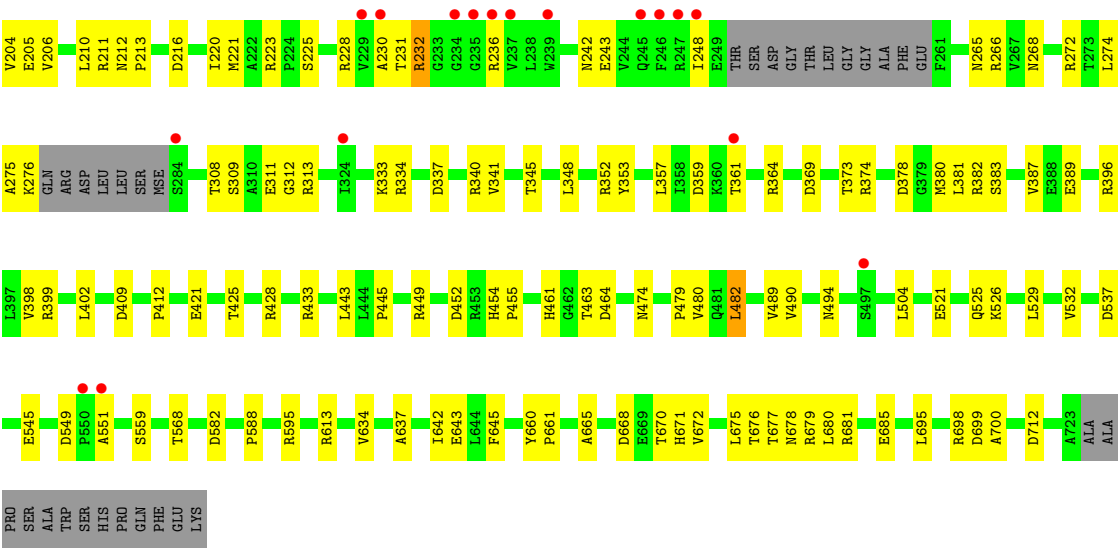
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl aminopeptidases/acylaminoacyl-peptidases-like protein



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.11Å 133.50Å 169.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.00 49.08 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.08-3.00) 100.0 (49.08-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10_2152	Depositor
R, R_{free}	0.237 , 0.259 (Not available) , 0.207	Depositor DCC
R_{free} test set	2606 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10681	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 2.54% 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: BGC

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	0.15	0/5501	0.35	0/7453
1	B	0.15	0/5370	0.35	0/7276
All	All	0.15	0/10871	0.35	0/14729

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5393	0	5316	109	0
1	B	5264	0	5193	108	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
All	All	10681	0	10533	203	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 10.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LYS:NZ	1:B:188:ASP:OD2	1.81	1.12
1:A:446:ARG:NH1	1:A:485:GLU:OE2	1.93	1.00
1:A:32:ARG:NH1	1:A:38:ASP:OD2	2.08	0.86
1:B:243:GLU:OE2	1:B:272:ARG:NH1	2.08	0.86
1:A:428:ARG:NH1	1:A:545:GLU:OE2	2.09	0.85
1:A:624:ASP:O	1:A:721:ARG:NH1	2.14	0.80
1:B:32:ARG:NH2	1:B:38:ASP:OD2	2.17	0.77
1:B:433:ARG:NH2	1:B:537:ASP:OD2	2.13	0.76
1:B:223:ARG:HH12	1:B:248:ILE:HB	1.48	0.76
1:A:243:GLU:OE2	1:A:272:ARG:NH2	2.21	0.73
1:B:220:ILE:HG22	1:B:221:MSE:HG3	1.69	0.72
1:A:302:ASP:OD2	1:A:319:ARG:NH2	2.24	0.70
1:A:200:SER:OG	1:B:199:ARG:NH2	2.28	0.67
1:B:169:LYS:HD2	1:B:213:PRO:HB3	1.77	0.66
1:A:305:LEU:HD13	1:A:363:VAL:HG11	1.78	0.65
1:A:677:THR:OG1	1:A:681:ARG:NH2	2.31	0.64
1:A:136:PRO:HB2	1:A:156:HIS:HB3	1.79	0.64
1:B:171:LEU:HB3	1:B:211:ARG:HB3	1.79	0.64
1:B:210:LEU:HB2	1:B:220:ILE:HD11	1.79	0.64
1:B:206:VAL:HG21	1:B:230:ALA:HB1	1.79	0.63
1:A:184:ARG:NH2	1:A:190:GLU:OE1	2.32	0.62
1:A:238:LEU:HD11	1:A:240:ARG:HH11	1.63	0.62
1:B:445:PRO:HD3	1:B:489:VAL:HG22	1.79	0.62
1:B:80:VAL:HG12	1:B:399:ARG:HD3	1.81	0.62
1:A:304:GLU:OE2	1:A:319:ARG:NE	2.26	0.62
1:A:364:ARG:NH2	1:A:405:ASP:OD1	2.26	0.61
1:B:120:ARG:HE	1:B:130:LEU:HD21	1.63	0.61
1:B:223:ARG:NH1	1:B:248:ILE:HB	2.14	0.61
1:B:480:VAL:HG13	1:B:490:VAL:HG11	1.81	0.61
1:A:358:ILE:HG12	1:A:363:VAL:HG12	1.80	0.61
1:B:352:ARG:NH1	1:B:369:ASP:O	2.33	0.61
1:A:181:ASP:OD2	1:A:182:GLY:N	2.32	0.61
1:B:364:ARG:NH2	1:B:402:LEU:O	2.34	0.61
1:B:670:THR:OG1	1:B:672:VAL:O	2.15	0.61
1:B:698:ARG:NH1	1:B:712:ASP:OD1	2.34	0.60
1:B:72:ARG:NH1	1:B:92:ASP:OD1	2.34	0.59
1:A:428:ARG:NH2	1:A:541:GLU:OE2	2.36	0.59
1:A:646:GLU:OE1	1:B:595:ARG:NH2	2.36	0.58
1:A:169:LYS:HB3	1:A:213:PRO:HG3	1.86	0.58
1:B:53:ASN:HD22	1:B:55:ARG:HB2	1.69	0.58
1:A:645:PHE:CZ	1:B:188:ASP:HB3	2.39	0.57
1:B:177:ARG:NH2	1:B:205:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:HIS:HB2	1:B:489:VAL:HG23	1.85	0.57
1:B:204:VAL:O	1:B:225:SER:OG	2.22	0.57
1:B:169:LYS:HB3	1:B:213:PRO:HG3	1.87	0.57
1:B:521:GLU:OE2	1:B:613:ARG:NE	2.36	0.56
1:A:199:ARG:NH2	1:A:665:ALA:O	2.37	0.56
1:A:122:ASP:OD2	1:A:126:LYS:HG2	2.05	0.56
1:B:396:ARG:HH12	1:B:412:PRO:HD3	1.70	0.56
1:A:250:THR:OG1	1:A:260:GLU:OE1	2.21	0.56
1:A:670:THR:OG1	1:A:672:VAL:O	2.20	0.56
1:A:341:VAL:HG22	1:A:358:ILE:HB	1.88	0.55
1:A:569:VAL:HG12	1:A:626:VAL:HG13	1.87	0.55
1:A:287:VAL:HG12	1:A:332:TRP:HZ2	1.71	0.55
1:A:525:GLN:HA	1:A:529:LEU:HB2	1.88	0.55
1:A:681:ARG:HH11	1:B:185:VAL:HG13	1.71	0.55
1:A:58:ILE:HG23	1:A:97:LEU:HD21	1.89	0.55
1:A:378:ASP:OD2	1:A:381:LEU:N	2.40	0.55
1:A:609:ASP:N	1:A:609:ASP:OD1	2.40	0.54
1:A:334:ARG:HG3	1:A:341:VAL:HG12	1.89	0.54
1:B:334:ARG:HG3	1:B:341:VAL:HG22	1.89	0.54
1:A:121:ILE:HG12	1:A:127:LEU:HB3	1.88	0.54
1:B:265:ASN:ND2	1:B:268:ASN:OD1	2.41	0.54
1:A:549:ASP:OD1	1:A:552:ARG:NH1	2.41	0.53
1:A:290:ARG:NH1	1:A:360:LYS:HG2	2.23	0.53
1:B:71:PRO:HG2	1:B:153:ARG:HH12	1.74	0.53
1:B:373:THR:HG21	1:B:389:GLU:OE2	2.08	0.53
1:B:212:ASN:HD21	1:B:216:ASP:HB2	1.74	0.53
1:A:152:ILE:HG13	1:A:153:ARG:H	1.74	0.53
1:A:378:ASP:OD1	1:A:383:SER:N	2.40	0.53
1:A:504:LEU:HD23	1:A:526:LYS:HB3	1.90	0.52
1:A:587:GLU:OE1	1:A:620:SER:OG	2.21	0.52
1:A:681:ARG:HH11	1:B:185:VAL:CG1	2.22	0.52
1:B:532:VAL:HG13	1:B:568:THR:HG23	1.91	0.52
1:A:280:LEU:O	1:A:284:SER:OG	2.18	0.52
1:B:425:THR:HG22	1:B:443:LEU:HD13	1.92	0.51
1:A:532:VAL:HG13	1:A:568:THR:HG22	1.92	0.51
1:A:706:ASP:OD2	1:A:706:ASP:N	2.44	0.51
1:A:480:VAL:HG13	1:A:490:VAL:HG11	1.91	0.51
1:A:72:ARG:NH1	1:A:90:THR:OG1	2.44	0.51
1:B:71:PRO:HG2	1:B:153:ARG:NH1	2.26	0.51
1:B:40:LEU:HD21	1:B:676:THR:HG23	1.93	0.51
1:A:52:ASP:OD1	1:A:336:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PRO:HG2	1:B:695:LEU:HD21	1.94	0.50
1:A:377:PHE:N	2:A:801:BGC:O1	2.30	0.50
1:A:568:THR:O	1:A:572:SER:N	2.44	0.50
1:B:479:PRO:HB2	1:B:482:LEU:HB2	1.94	0.50
1:B:699:ASP:OD1	1:B:700:ALA:N	2.45	0.50
1:A:175:GLN:HG2	1:A:209:PHE:HE1	1.77	0.50
1:A:698:ARG:NH2	1:A:712:ASP:OD2	2.37	0.50
1:B:525:GLN:HA	1:B:529:LEU:HB2	1.94	0.50
1:A:326:ASP:O	1:A:329:SER:OG	2.26	0.49
1:A:287:VAL:HG12	1:A:332:TRP:CZ2	2.46	0.49
1:A:522:THR:O	1:A:526:LYS:HG2	2.12	0.49
1:B:106:TRP:HB2	1:B:121:ILE:HB	1.95	0.49
1:A:192:THR:HG22	1:B:642:ILE:HG23	1.95	0.49
1:B:78:VAL:HG22	1:B:85:THR:HG22	1.94	0.48
1:A:223:ARG:HH22	1:A:250:THR:HG22	1.78	0.48
1:A:456:ALA:HB3	1:A:553:VAL:HG23	1.95	0.48
1:B:588:PRO:HD2	1:B:643:GLU:OE2	2.13	0.48
1:A:479:PRO:HB2	1:A:482:LEU:HB3	1.95	0.48
1:B:189:GLU:H	1:B:189:GLU:CD	2.21	0.48
1:A:144:MSE:HE1	1:B:665:ALA:HB3	1.96	0.48
1:B:309:SER:OG	1:B:313:ARG:N	2.41	0.48
1:A:660:TYR:HA	1:B:185:VAL:HG12	1.95	0.48
1:B:504:LEU:HD23	1:B:526:LYS:HG3	1.96	0.48
1:B:428:ARG:HH22	1:B:545:GLU:CD	2.22	0.47
1:A:139:VAL:O	1:A:154:PRO:HA	2.13	0.47
1:A:493:LEU:HD23	1:A:535:PHE:HD1	1.78	0.47
1:B:634:VAL:HG12	1:B:637:ALA:H	1.79	0.47
1:A:41:THR:HG21	1:A:416:ARG:NH1	2.30	0.47
1:B:464:ASP:HB3	1:B:474:ASN:HB2	1.96	0.47
1:B:559:SER:HB2	1:B:671:HIS:NE2	2.29	0.47
1:B:188:ASP:O	1:B:192:THR:HG23	2.15	0.47
1:B:170:TRP:CD2	1:B:213:PRO:HD3	2.50	0.47
1:A:428:ARG:HH12	1:A:545:GLU:CD	2.11	0.47
1:B:228:ARG:HE	1:B:232:ARG:HH21	1.61	0.47
1:B:461:HIS:ND1	1:B:464:ASP:OD1	2.45	0.47
1:A:290:ARG:HB2	1:A:307:GLU:CD	2.40	0.47
1:A:143:ASP:OD2	1:B:200:SER:OG	2.32	0.47
1:A:290:ARG:HH12	1:A:360:LYS:HG2	1.80	0.47
1:B:378:ASP:OD2	1:B:383:SER:N	2.47	0.46
1:B:582:ASP:HB3	1:B:671:HIS:CE1	2.50	0.46
1:A:645:PHE:HZ	1:B:188:ASP:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PHE:O	1:A:191:VAL:HG23	2.15	0.46
1:A:304:GLU:CD	1:A:319:ARG:HE	2.20	0.46
1:A:578:ALA:N	1:A:629:ALA:O	2.41	0.46
1:B:45:VAL:O	1:B:374:ARG:HG3	2.15	0.46
1:A:221:MSE:SE	1:A:262:VAL:HG11	2.65	0.46
1:B:677:THR:O	1:B:681:ARG:HG2	2.15	0.46
1:A:661:PRO:HD3	1:B:185:VAL:HG12	1.98	0.46
1:A:465:ALA:O	1:A:494:ASN:ND2	2.36	0.46
1:B:31:GLY:HA3	1:B:421:GLU:HB2	1.98	0.46
1:B:676:THR:O	1:B:680:LEU:HB2	2.15	0.46
1:A:71:PRO:HD3	1:A:674:TYR:O	2.16	0.45
1:A:171:LEU:HB3	1:A:211:ARG:HB3	1.98	0.45
1:A:218:THR:HG21	1:A:269:ARG:NH1	2.31	0.45
1:A:626:VAL:O	1:A:721:ARG:NH2	2.49	0.45
1:A:212:ASN:HD21	1:A:216:ASP:HB2	1.82	0.45
1:B:242:ASN:O	1:B:266:ARG:HG2	2.17	0.45
1:B:333:LYS:HG2	1:B:381:LEU:HD11	1.97	0.45
1:B:359:ASP:OD2	1:B:361:THR:HB	2.17	0.45
1:A:198:ARG:NH2	1:B:195:LEU:O	2.49	0.45
1:A:198:ARG:HA	1:A:198:ARG:HD2	1.84	0.45
1:A:576:ARG:HD3	1:A:694:LEU:HA	1.98	0.45
1:B:45:VAL:HG12	1:B:60:ALA:O	2.16	0.45
1:A:453:ARG:NH1	1:A:546:GLY:HA2	2.32	0.45
1:B:143:ASP:OD1	1:B:199:ARG:NH2	2.47	0.45
1:A:286:LEU:HD11	1:A:325:GLY:HA3	1.99	0.45
1:A:317:TYR:HD1	1:A:362:GLY:HA2	1.81	0.45
1:B:228:ARG:HD2	1:B:232:ARG:HD3	1.99	0.45
1:B:45:VAL:HG21	1:B:387:VAL:HG21	1.97	0.45
1:A:692:TYR:OH	1:A:712:ASP:OD1	2.24	0.44
1:B:340:ARG:NH2	1:B:357:LEU:HD21	2.32	0.44
1:B:357:LEU:HD23	1:B:364:ARG:HH22	1.83	0.44
1:A:497:SER:O	1:A:500:GLN:HG2	2.18	0.44
1:A:677:THR:O	1:A:681:ARG:HG3	2.18	0.44
1:B:66:LEU:HD13	1:B:676:THR:HG21	1.99	0.43
1:B:170:TRP:CE3	1:B:212:ASN:HA	2.53	0.43
1:B:398:VAL:HG12	1:B:409:ASP:HA	2.00	0.43
1:B:660:TYR:OH	1:B:685:GLU:OE1	2.28	0.43
1:A:43:PRO:HG3	1:A:414:SER:HB2	2.01	0.43
1:A:304:GLU:CD	1:A:319:ARG:HH11	2.19	0.43
1:B:186:ARG:HB3	1:B:190:GLU:HB2	2.01	0.43
1:B:396:ARG:HD3	1:B:409:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD13	1:A:176:LEU:HD11	2.00	0.43
1:A:153:ARG:HD3	1:A:674:TYR:CD1	2.54	0.43
1:A:40:LEU:HD22	1:A:680:LEU:HD21	2.01	0.43
1:A:229:VAL:HG21	1:A:247:ARG:HG3	2.00	0.43
1:A:238:LEU:HB3	1:A:245:GLN:HB3	2.01	0.43
1:A:305:LEU:HD12	1:A:320:VAL:HG11	2.01	0.43
1:A:322:PHE:HA	1:A:347:GLY:HA2	2.01	0.43
1:A:416:ARG:O	1:A:419:GLU:HG2	2.18	0.43
1:A:453:ARG:CZ	1:A:546:GLY:HA2	2.49	0.43
1:B:274:LEU:HD12	1:B:275:ALA:O	2.18	0.43
1:A:188:ASP:HB3	1:B:645:PHE:CZ	2.55	0.42
1:A:248:ILE:HG12	1:A:262:VAL:HG23	2.00	0.42
1:B:463:THR:HA	1:B:494:ASN:CG	2.44	0.42
1:B:152:ILE:HG13	1:B:153:ARG:O	2.19	0.42
1:B:187:PHE:O	1:B:191:VAL:HG23	2.19	0.42
1:B:308:THR:HG23	1:B:312:GLY:HA2	2.01	0.42
1:A:455:PRO:HG3	1:A:695:LEU:HD21	2.02	0.42
1:A:493:LEU:HD23	1:A:535:PHE:CD1	2.54	0.42
1:B:463:THR:HG22	1:B:494:ASN:HB3	2.02	0.42
1:B:199:ARG:HE	1:B:668:ASP:CG	2.27	0.41
1:B:337:ASP:HB2	1:B:380:MSE:SE	2.70	0.41
1:A:152:ILE:HD12	1:A:152:ILE:HA	1.87	0.41
1:A:453:ARG:NH2	1:A:543:ALA:O	2.53	0.41
1:B:675:LEU:O	1:B:679:ARG:HG2	2.20	0.41
1:A:437:TRP:HZ3	1:A:439:SER:HB3	1.85	0.41
1:A:117:GLN:HB2	1:A:119:TYR:HE2	1.85	0.41
1:B:53:ASN:ND2	1:B:55:ARG:HB2	2.34	0.41
1:B:86:LYS:HE3	1:B:86:LYS:HB2	1.95	0.41
1:B:378:ASP:CG	1:B:382:ARG:H	2.27	0.41
1:B:449:ARG:HB2	1:B:452:ASP:OD2	2.20	0.41
1:B:549:ASP:OD2	1:B:549:ASP:C	2.63	0.41
1:B:675:LEU:HD23	1:B:675:LEU:HA	1.84	0.41
1:B:160:LEU:HD21	1:B:231:THR:O	2.21	0.41
1:B:549:ASP:OD2	1:B:551:ALA:N	2.40	0.41
1:A:199:ARG:NH2	1:A:667:SER:O	2.54	0.41
1:B:345:THR:O	1:B:353:TYR:HA	2.21	0.41
1:B:162:TYR:HA	1:B:173:TYR:HA	2.04	0.40
1:B:661:PRO:O	1:B:678:ASN:ND2	2.52	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	691/756 (91%)	663 (96%)	28 (4%)	0	100	100
1	B	671/756 (89%)	646 (96%)	25 (4%)	0	100	100
All	All	1362/1512 (90%)	1309 (96%)	53 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	565/598 (94%)	553 (98%)	12 (2%)	47	75
1	B	552/598 (92%)	544 (99%)	8 (1%)	59	80
All	All	1117/1196 (93%)	1097 (98%)	20 (2%)	51	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	135	ASN
1	A	137	VAL
1	A	139	VAL
1	A	198	ARG
1	A	304	GLU
1	A	319	ARG
1	A	348	LEU

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Mol	Chain	Res	Type
1	A	357	LEU
1	A	364	ARG
1	A	399	ARG
1	A	512	LEU
1	B	152	ILE
1	B	192	THR
1	B	232	ARG
1	B	236	ARG
1	B	276	LYS
1	B	311	GLU
1	B	348	LEU
1	B	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	135	ASN
1	A	156	HIS
1	A	245	GLN
1	A	622	ASN
1	A	717	ASN
1	B	686	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	B	801	-	12,12,12	0.53	0	17,17,17	0.47	0
2	BGC	A	801	-	12,12,12	0.54	0	17,17,17	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	801	-	-	1/2/22/22	0/1/1/1
2	BGC	A	801	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BGC	O5-C5-C6-O6
2	B	801	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BGC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	685/756 (90%)	0.14	10 (1%)	72 49	55, 77, 104, 137	0
1	B	668/756 (88%)	0.21	20 (2%)	52 30	52, 75, 113, 165	0
All	All	1353/1512 (89%)	0.17	30 (2%)	62 39	52, 76, 110, 165	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	GLY	4.3
1	A	253	GLY	3.9
1	B	284	SER	3.8
1	A	151	GLY	3.5
1	B	235	GLY	3.4
1	A	152	ILE	3.1
1	A	409	ASP	3.0
1	B	236	ARG	2.9
1	B	229	VAL	2.8
1	B	237	VAL	2.8
1	B	230	ALA	2.8
1	B	361	THR	2.8
1	A	726	PRO	2.6
1	B	234	GLY	2.6
1	B	246	PHE	2.5
1	B	550	PRO	2.5
1	B	239	TRP	2.4
1	A	725	ALA	2.4
1	B	245	GLN	2.3
1	A	273	THR	2.3
1	B	174	SER	2.3
1	A	150	GLY	2.2
1	B	247	ARG	2.2
1	B	497	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	171	LEU	2.1
1	B	324	ILE	2.1
1	A	275	ALA	2.1
1	A	279	ASP	2.1
1	B	248	ILE	2.0
1	B	551	ALA	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($\text{\AA}^2$)	Q<0.9
2	BGC	A	801	12/12	0.74	0.12	88,93,99,102	0
2	BGC	B	801	12/12	0.81	0.11	93,97,103,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.