



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:41 PM UTC

PDB ID : 5ES9 / pdb_00005es9
Title : Crystal structure of the LgrA initiation module in the formylation state
Authors : Reimer, J.M.; Aloise, M.N.; Schmeing, T.M.
Deposited on : 2015-11-16
Resolution : 3.77 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

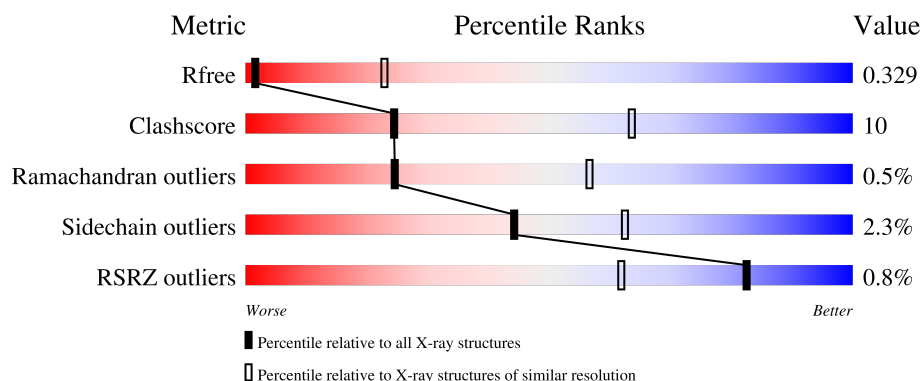
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.77 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	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)

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	776	73% 24% ..
1	B	776	68% 19% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11509 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.

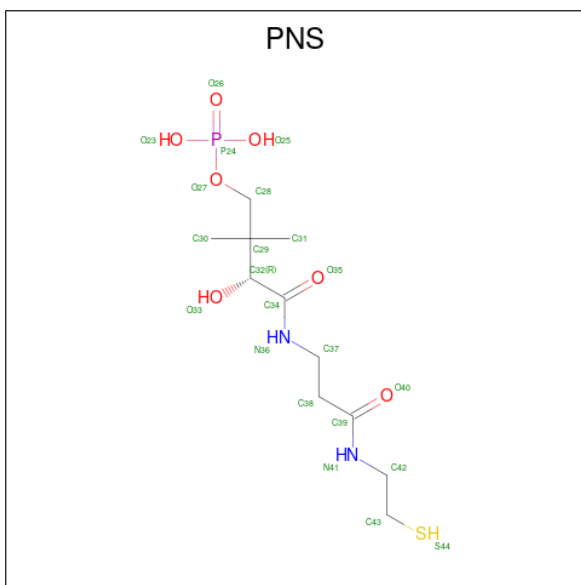
- Molecule 1 is a protein called Linear gramicidin synthetase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			6064	3869	1042	1126	27			
1	B	681	Total	C	N	O	S	0	0	0
			5440	3473	930	1012	25			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	768	ALA	-	expression tag	UNP Q70LM7
A	769	ALA	-	expression tag	UNP Q70LM7
A	770	ALA	-	expression tag	UNP Q70LM7
A	771	GLU	-	expression tag	UNP Q70LM7
A	772	ASN	-	expression tag	UNP Q70LM7
A	773	LEU	-	expression tag	UNP Q70LM7
A	774	TYR	-	expression tag	UNP Q70LM7
A	775	PHE	-	expression tag	UNP Q70LM7
A	776	GLN	-	expression tag	UNP Q70LM7
B	1	MET	-	initiating methionine	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	768	ALA	-	expression tag	UNP Q70LM7
B	769	ALA	-	expression tag	UNP Q70LM7
B	770	ALA	-	expression tag	UNP Q70LM7
B	771	GLU	-	expression tag	UNP Q70LM7
B	772	ASN	-	expression tag	UNP Q70LM7
B	773	LEU	-	expression tag	UNP Q70LM7
B	774	TYR	-	expression tag	UNP Q70LM7
B	775	PHE	-	expression tag	UNP Q70LM7
B	776	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

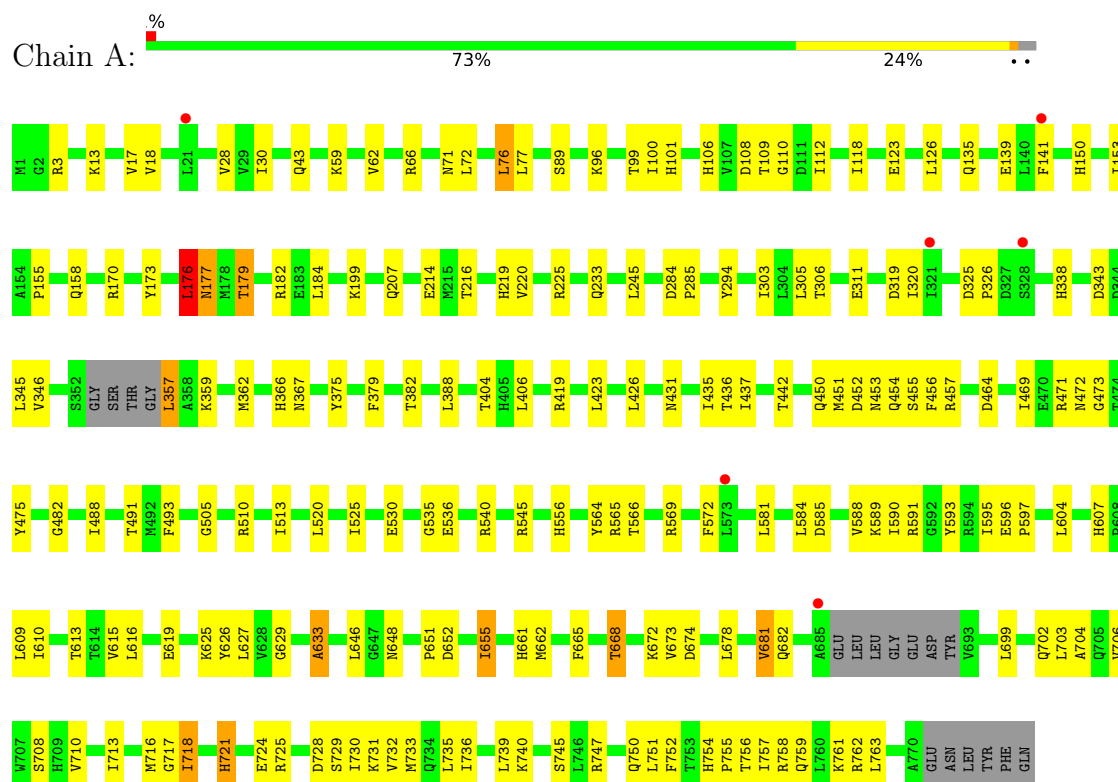


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			5	1	3	1		

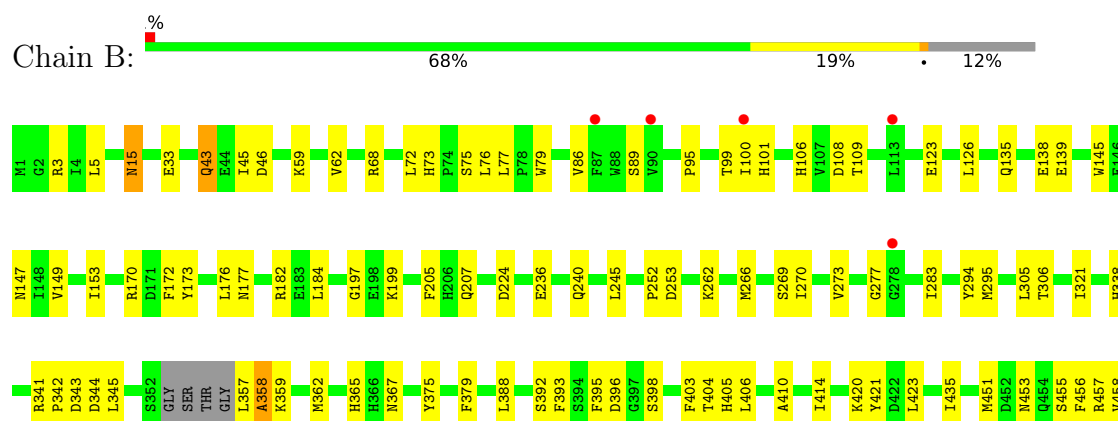
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Linear gramicidin synthetase subunit A



• Molecule 1: Linear gramicidin synthetase subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.06Å 162.06Å 206.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.77 48.45 – 3.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.45-3.77) 99.9 (48.45-3.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.308 , 0.331 0.311 , 0.329	Depositor DCC
R_{free} test set	2013 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	188.6	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 226.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.207 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11509	wwPDB-VP
Average B, all atoms (Å ²)	261.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: PNS

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	0.38	1/6203 (0.0%)	0.81	8/8418 (0.1%)
1	B	0.34	0/5568	0.81	8/7559 (0.1%)
All	All	0.36	1/11771 (0.0%)	0.81	16/15977 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	LEU	C-O	-5.67	1.16	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	GLY	N-CA-C	6.81	120.54	110.60
1	B	463	GLY	N-CA-C	-6.69	106.73	114.69
1	A	176	LEU	N-CA-C	6.05	120.28	113.02
1	A	633	ALA	N-CA-C	6.04	113.66	108.22
1	B	556	HIS	CA-C-N	5.66	125.13	119.24
1	B	556	HIS	C-N-CA	5.66	125.13	119.24
1	A	482	GLY	CA-C-N	5.60	125.91	119.92
1	A	482	GLY	C-N-CA	5.60	125.91	119.92
1	B	535	GLY	N-CA-C	5.57	117.94	110.43
1	B	596	GLU	CA-C-N	5.39	125.47	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	GLU	C-N-CA	5.39	125.47	119.32
1	B	633	ALA	N-CA-C	5.35	113.04	108.22
1	A	176	LEU	CA-C-N	-5.27	114.38	122.60
1	A	176	LEU	C-N-CA	-5.27	114.38	122.60
1	A	306	THR	N-CA-C	5.01	115.91	108.60
1	B	306	THR	N-CA-C	5.01	115.91	108.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6064	0	6001	136	1
1	B	5440	0	5369	97	0
2	A	5	0	0	0	0
All	All	11509	0	11370	227	1

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 (227) 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:455:SER:O	1:B:199:LYS:NZ	2.00	0.94
1:B:453:ASN:HD21	1:B:456:PHE:H	1.19	0.91
1:A:126:LEU:HD12	1:A:177:ASN:HA	1.55	0.87
1:A:216:THR:HB	1:A:219:HIS:HD2	1.40	0.86
1:A:588:VAL:HG21	1:A:625:LYS:HD2	1.60	0.82
1:A:713:ILE:HD11	1:A:725:ARG:HG2	1.65	0.78
1:B:668:THR:HG23	1:B:674:ASP:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:HD21	1:A:456:PHE:H	1.32	0.77
1:B:199:LYS:O	1:B:510:ARG:NH2	2.19	0.76
1:B:681:VAL:HG12	1:B:682:GLN:H	1.51	0.75
1:A:199:LYS:O	1:A:510:ARG:NH2	2.19	0.75
1:A:3:ARG:NH1	1:A:43:GLN:O	2.21	0.74
1:A:652:ASP:HB2	1:A:758:ARG:HD3	1.70	0.74
1:B:482:GLY:HA3	1:B:489:MET:HA	1.68	0.74
1:A:590:ILE:HG13	1:A:627:LEU:HG	1.70	0.73
1:B:126:LEU:HD11	1:B:184:LEU:HD22	1.72	0.71
1:B:3:ARG:NH1	1:B:43:GLN:O	2.25	0.70
1:B:615:VAL:HG12	1:B:629:GLY:HA2	1.73	0.69
1:A:615:VAL:HG12	1:A:629:GLY:HA2	1.75	0.68
1:B:77:LEU:HB2	1:B:99:THR:HG21	1.76	0.68
1:A:589:LYS:HB2	1:A:593:TYR:O	1.93	0.68
1:A:648:ASN:HA	1:A:762:ARG:HH12	1.60	0.67
1:A:367:ASN:ND2	1:A:536:GLU:O	2.28	0.66
1:A:730:ILE:HG13	1:A:731:LYS:HD2	1.78	0.65
1:A:177:ASN:N	1:A:177:ASN:ND2	2.43	0.65
1:A:588:VAL:HG12	1:A:589:LYS:O	1.95	0.65
1:A:708:SER:OG	1:A:713:ILE:O	2.15	0.64
1:A:77:LEU:HD21	1:A:108:ASP:O	1.99	0.63
1:B:396:ASP:HB2	1:B:488:ILE:HG12	1.80	0.63
1:A:177:ASN:HD22	1:A:177:ASN:H	1.47	0.62
1:B:510:ARG:NH1	1:B:536:GLU:OE1	2.32	0.62
1:A:754:HIS:HB3	1:A:759:GLN:HB3	1.80	0.62
1:B:595:ILE:HG21	1:B:627:LEU:HD11	1.80	0.62
1:B:665:PHE:HD2	1:B:673:VAL:HG11	1.64	0.61
1:A:668:THR:HG23	1:A:674:ASP:HB3	1.83	0.60
1:A:740:LYS:HD3	1:A:745:SER:HB2	1.82	0.60
1:A:718:ILE:HG13	1:A:758:ARG:HB3	1.84	0.59
1:B:435:ILE:O	1:B:455:SER:OG	2.20	0.59
1:B:77:LEU:HD11	1:B:108:ASP:HB3	1.85	0.59
1:A:177:ASN:N	1:A:177:ASN:HD22	2.01	0.58
1:A:721:HIS:CD2	1:A:755:PRO:HB2	2.37	0.58
1:A:747:ARG:HB3	1:A:750:GLN:HG2	1.85	0.58
1:A:665:PHE:HD2	1:A:673:VAL:HG11	1.67	0.58
1:B:170:ARG:NH2	1:B:177:ASN:OD1	2.37	0.58
1:B:207:GLN:HG2	1:B:338:HIS:CE1	2.38	0.58
1:A:388:LEU:HD13	1:A:435:ILE:HG21	1.86	0.57
1:B:392:SER:HB3	1:B:395:PHE:CE2	2.39	0.57
1:A:454:GLN:HG2	1:B:197:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD12	1:B:95:PRO:HB2	1.87	0.56
1:B:379:PHE:O	1:B:457:ARG:NH1	2.38	0.56
1:A:216:THR:HB	1:A:219:HIS:CD2	2.30	0.56
1:A:442:THR:HB	1:A:464:ASP:HB2	1.88	0.56
1:A:345:LEU:HD11	1:A:362:MET:HE2	1.87	0.55
1:A:18:VAL:HG13	1:A:28:VAL:HG11	1.88	0.55
1:B:367:ASN:HB3	1:B:487:THR:OG1	2.07	0.55
1:A:590:ILE:HB	1:A:595:ILE:HD12	1.88	0.55
1:B:610:ILE:HG22	1:B:633:ALA:HB2	1.89	0.55
1:A:219:HIS:ND1	1:B:341:ARG:HD2	2.22	0.55
1:A:758:ARG:O	1:A:762:ARG:HG3	2.08	0.54
1:B:73:HIS:ND1	1:B:75:SER:OG	2.39	0.54
1:A:106:HIS:HB2	1:A:109:THR:OG1	2.08	0.54
1:B:388:LEU:HD13	1:B:435:ILE:HG21	1.90	0.54
1:A:343:ASP:O	1:A:540:ARG:NH2	2.41	0.54
1:A:135:GLN:NE2	1:A:139:GLU:OE2	2.40	0.54
1:B:528:ALA:HA	1:B:571:ARG:HB3	1.89	0.54
1:A:303:ILE:HD13	1:A:319:ASP:HB2	1.91	0.53
1:B:283:ILE:HG12	1:B:295:MET:HE2	1.89	0.53
1:A:721:HIS:ND1	1:A:724:GLU:OE1	2.41	0.53
1:A:736:ILE:HA	1:A:739:LEU:HG	1.90	0.53
1:B:662:MET:HE1	1:B:678:LEU:HD22	1.91	0.53
1:A:651:PRO:HB3	1:A:756:THR:HG21	1.91	0.53
1:B:457:ARG:HD2	1:B:458:VAL:HG23	1.91	0.53
1:A:123:GLU:HG2	1:A:182:ARG:HH12	1.72	0.52
1:A:375:TYR:CD1	1:A:404:THR:HB	2.44	0.52
1:A:759:GLN:HA	1:A:762:ARG:HE	1.74	0.52
1:A:454:GLN:CG	1:B:197:GLY:HA2	2.40	0.52
1:A:652:ASP:HA	1:A:655:ILE:HD13	1.92	0.52
1:A:126:LEU:HD11	1:A:184:LEU:HD22	1.90	0.52
1:A:366:HIS:ND1	1:A:536:GLU:OE2	2.34	0.52
1:B:46:ASP:O	1:B:68:ARG:HD2	2.10	0.52
1:A:610:ILE:HG22	1:A:633:ALA:HB2	1.91	0.51
1:A:13:LYS:HG2	1:A:30:ILE:HG21	1.93	0.51
1:B:507:PRO:HG3	1:B:513:ILE:HD12	1.92	0.51
1:B:496:ASP:OD1	1:B:496:ASP:N	2.38	0.50
1:B:665:PHE:CD2	1:B:673:VAL:HG11	2.45	0.50
1:A:379:PHE:O	1:A:457:ARG:NH1	2.42	0.50
1:B:473:GLY:HA3	1:B:475:TYR:CE2	2.46	0.50
1:B:604:LEU:HD13	1:B:646:LEU:HD11	1.93	0.50
1:A:471:ARG:HD2	1:A:475:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:NE2	1:B:139:GLU:OE2	2.44	0.50
1:B:604:LEU:O	1:B:610:ILE:HD11	2.11	0.50
1:B:173:TYR:HB3	1:B:176:LEU:HD12	1.93	0.50
1:A:604:LEU:HD13	1:A:646:LEU:HD11	1.93	0.50
1:A:423:LEU:HB2	1:A:451:MET:HE3	1.94	0.50
1:A:493:PHE:HB2	1:A:505:GLY:HA3	1.93	0.50
1:A:220:VAL:HB	1:B:341:ARG:HH22	1.76	0.49
1:A:728:ASP:O	1:A:732:VAL:HG13	2.12	0.49
1:A:245:LEU:HD21	1:A:305:LEU:HD11	1.93	0.49
1:A:595:ILE:HG21	1:A:627:LEU:HD11	1.94	0.49
1:A:699:LEU:O	1:A:702:GLN:HG2	2.12	0.49
1:A:713:ILE:CD1	1:A:725:ARG:HG2	2.40	0.49
1:A:750:GLN:HB3	1:A:763:LEU:HD13	1.95	0.49
1:A:110:GLY:O	1:A:158:GLN:NE2	2.37	0.49
1:A:294:TYR:OH	1:A:545:ARG:NH2	2.46	0.49
1:A:732:VAL:HB	1:A:751:LEU:HD23	1.93	0.49
1:B:252:PRO:O	1:B:253:ASP:HB2	2.11	0.49
1:A:153:ILE:O	1:A:155:PRO:HD3	2.12	0.49
1:A:718:ILE:HD11	1:A:758:ARG:HD2	1.94	0.48
1:B:172:PHE:CZ	1:B:522:LEU:HG	2.48	0.48
1:A:730:ILE:HA	1:A:733:MET:HE3	1.94	0.48
1:B:73:HIS:HD1	1:B:75:SER:HG	1.62	0.48
1:A:431:ASN:HA	1:A:455:SER:HB2	1.95	0.48
1:B:345:LEU:HD11	1:B:362:MET:HE2	1.94	0.48
1:B:471:ARG:HD2	1:B:475:TYR:CE1	2.48	0.48
1:A:633:ALA:HB3	1:A:661:HIS:HD2	1.79	0.48
1:A:170:ARG:HH21	1:A:177:ASN:HB3	1.79	0.48
1:B:86:VAL:O	1:B:89:SER:HB3	2.15	0.47
1:A:89:SER:O	1:A:96:LYS:NZ	2.46	0.47
1:A:604:LEU:O	1:A:610:ILE:HD11	2.14	0.47
1:A:604:LEU:HG	1:A:613:THR:HG21	1.96	0.47
1:A:735:LEU:HD23	1:A:751:LEU:HD22	1.97	0.47
1:B:343:ASP:O	1:B:540:ARG:NH2	2.44	0.47
1:B:639:HIS:HE1	1:B:643:ARG:HD2	1.79	0.47
1:A:96:LYS:HB2	1:A:118:ILE:O	2.15	0.46
1:B:59:LYS:O	1:B:62:VAL:HG12	2.15	0.46
1:A:704:ALA:HB1	1:A:716:MET:HB2	1.96	0.46
1:A:59:LYS:O	1:A:62:VAL:HG12	2.16	0.46
1:A:173:TYR:HB3	1:A:176:LEU:HD12	1.98	0.46
1:A:739:LEU:HD12	1:A:740:LYS:N	2.31	0.46
1:A:520:LEU:O	1:A:556:HIS:NE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLU:HG2	1:B:182:ARG:HH12	1.80	0.46
1:B:270:ILE:HD11	1:B:393:PHE:HE1	1.81	0.46
1:B:147:ASN:HB3	1:B:153:ILE:HD11	1.97	0.46
1:A:357:LEU:HB2	1:A:359:LYS:HZ1	1.81	0.46
1:B:15:ASN:ND2	1:B:138:GLU:OE2	2.49	0.46
1:A:652:ASP:CB	1:A:758:ARG:HD3	2.45	0.45
1:B:106:HIS:HB2	1:B:109:THR:OG1	2.17	0.45
1:A:590:ILE:HD12	1:A:626:TYR:HA	1.99	0.45
1:A:706:VAL:O	1:A:710:VAL:HG23	2.16	0.45
1:B:485:GLU:OE1	1:B:485:GLU:N	2.47	0.45
1:A:589:LYS:O	1:A:590:ILE:HG12	2.17	0.45
1:B:77:LEU:HD22	1:B:101:HIS:CG	2.52	0.45
1:A:569:ARG:HB3	1:A:581:LEU:O	2.17	0.45
1:B:672:LYS:HG2	1:B:673:VAL:HG13	1.98	0.45
1:A:678:LEU:HD12	1:A:678:LEU:HA	1.81	0.45
1:A:473:GLY:HA3	1:A:475:TYR:CE2	2.51	0.45
1:A:681:VAL:HG12	1:A:682:GLN:H	1.82	0.45
1:A:596:GLU:HA	1:A:597:PRO:HD2	1.80	0.44
1:B:245:LEU:HD21	1:B:305:LEU:HD11	1.98	0.44
1:B:573:LEU:HB2	1:B:577:ASN:O	2.17	0.44
1:B:453:ASN:OD1	1:B:455:SER:HB3	2.17	0.44
1:A:99:THR:HG21	1:A:112:ILE:HG12	1.99	0.44
1:A:450:GLN:O	1:A:472:ASN:ND2	2.51	0.44
1:A:170:ARG:NH2	1:A:177:ASN:HB3	2.31	0.44
1:A:452:ASP:HA	1:A:472:ASN:HB2	2.00	0.44
1:A:619:GLU:HG3	1:A:625:LYS:NZ	2.33	0.44
1:A:325:ASP:HA	1:A:326:PRO:HD2	1.89	0.44
1:B:596:GLU:HA	1:B:597:PRO:HD2	1.75	0.44
1:A:590:ILE:HG22	1:A:591:ARG:HB2	1.99	0.44
1:B:375:TYR:CD1	1:B:404:THR:HB	2.53	0.44
1:B:73:HIS:NE2	1:B:108:ASP:OD2	2.51	0.43
1:A:525:ILE:HG23	1:A:572:PHE:HB3	2.00	0.43
1:A:728:ASP:H	1:A:731:LYS:HB2	1.82	0.43
1:A:699:LEU:HB2	1:A:761:LYS:HE3	2.00	0.43
1:B:73:HIS:O	1:B:75:SER:N	2.47	0.43
1:B:341:ARG:HD3	1:B:343:ASP:OD1	2.18	0.43
1:B:405:HIS:HB3	1:B:410:ALA:HB3	2.01	0.43
1:B:681:VAL:HG12	1:B:682:GLN:N	2.28	0.43
1:A:758:ARG:HA	1:A:761:LYS:HB3	2.01	0.43
1:B:478:TYR:HB3	1:B:492:MET:SD	2.58	0.43
1:A:750:GLN:HB3	1:A:763:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.83	0.43
1:B:342:PRO:HA	1:B:365:HIS:HB2	2.01	0.43
1:A:71:ASN:HB3	1:A:101:HIS:NE2	2.33	0.43
1:A:724:GLU:OE1	1:A:724:GLU:N	2.52	0.43
1:A:112:ILE:O	1:A:155:PRO:HA	2.19	0.43
1:A:179:THR:CG2	1:A:184:LEU:HB2	2.49	0.43
1:A:732:VAL:O	1:A:736:ILE:HG12	2.18	0.43
1:A:732:VAL:HG11	1:A:752:PHE:HE1	1.84	0.43
1:B:252:PRO:HA	1:B:277:GLY:O	2.18	0.43
1:B:423:LEU:HB2	1:B:451:MET:HE3	2.00	0.43
1:A:72:LEU:HD22	1:A:100:ILE:HG12	2.01	0.42
1:A:530:GLU:OE1	1:A:565:ARG:NH1	2.52	0.42
1:A:564:TYR:CE2	1:A:566:THR:HA	2.54	0.42
1:A:717:GLY:O	1:A:757:ILE:HG13	2.19	0.42
1:B:392:SER:HB3	1:B:395:PHE:CD2	2.53	0.42
1:A:763:LEU:HA	1:A:763:LEU:HD23	1.78	0.42
1:B:456:PHE:O	1:B:475:TYR:HB3	2.19	0.42
1:A:207:GLN:HG2	1:A:338:HIS:CE1	2.54	0.42
1:B:262:LYS:HD3	1:B:266:MET:HE1	2.01	0.42
1:B:420:LYS:HG2	1:B:421:TYR:CD1	2.54	0.42
1:A:607:HIS:CE1	1:A:609:LEU:HB2	2.54	0.42
1:B:5:LEU:HB2	1:B:45:ILE:HD12	2.02	0.42
1:B:345:LEU:HD21	1:B:362:MET:HB3	2.01	0.42
1:A:436:THR:OG1	1:A:437:ILE:HG22	2.19	0.42
1:A:703:LEU:O	1:A:706:VAL:HG12	2.20	0.42
1:B:72:LEU:HD22	1:B:100:ILE:HG12	2.01	0.42
1:A:456:PHE:O	1:A:475:TYR:HB3	2.19	0.42
1:A:17:VAL:HG13	1:A:141:PHE:CE1	2.55	0.42
1:A:419:ARG:O	1:A:426:LEU:HB2	2.20	0.42
1:B:205:PHE:CE1	1:B:403:PHE:HB3	2.55	0.42
1:A:732:VAL:HG11	1:A:752:PHE:CE1	2.55	0.41
1:B:269:SER:O	1:B:273:VAL:HG23	2.20	0.41
1:B:294:TYR:HE2	1:B:358:ALA:HB1	1.85	0.41
1:A:729:SER:O	1:A:732:VAL:HG22	2.21	0.41
1:B:534:VAL:HG22	1:B:563:MET:HG2	2.01	0.41
1:B:632:VAL:HA	1:B:662:MET:O	2.21	0.41
1:A:219:HIS:HE1	1:B:344:ASP:OD1	2.03	0.41
1:B:236:GLU:O	1:B:240:GLN:HG3	2.21	0.41
1:B:655:ILE:HA	1:B:656:PRO:HD3	1.88	0.41
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.86	0.41
1:B:493:PHE:CZ	1:B:503:PRO:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:HA	1:A:285:PRO:HD3	1.92	0.41
1:A:493:PHE:HB2	1:A:505:GLY:CA	2.49	0.41
1:B:76:LEU:O	1:B:79:TRP:N	2.54	0.41
1:B:145:TRP:O	1:B:149:VAL:HG23	2.21	0.41
1:B:392:SER:O	1:B:398:SER:HB2	2.20	0.41
1:B:512:ARG:NH2	1:B:561:GLU:OE2	2.51	0.41
1:A:627:LEU:HD23	1:A:627:LEU:HA	1.87	0.41
1:B:33:GLU:N	1:B:33:GLU:OE2	2.54	0.41
1:A:311:GLU:HG3	1:A:320:ILE:HD13	2.02	0.40
1:A:359:LYS:HD3	1:A:545:ARG:NH1	2.36	0.40
1:A:662:MET:HE3	1:A:665:PHE:CE1	2.56	0.40
1:B:224:ASP:HB2	1:B:414:ILE:HG13	2.02	0.40
1:B:420:LYS:HG2	1:B:421:TYR:CE1	2.57	0.40
1:A:616:LEU:HD11	1:A:678:LEU:HD23	2.03	0.40
1:A:77:LEU:HB2	1:A:99:THR:CB	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:O	1:A:233:GLN:NE2[5_547]	2.15	0.05

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	753/776 (97%)	716 (95%)	33 (4%)	4 (0%)	24 56
1	B	677/776 (87%)	648 (96%)	26 (4%)	3 (0%)	30 61
All	All	1430/1552 (92%)	1364 (95%)	59 (4%)	7 (0%)	24 56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	584	LEU
1	A	585	ASP
1	A	76	LEU
1	B	488	ILE
1	A	488	ILE
1	B	358	ALA
1	B	681	VAL

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	652/666 (98%)	634 (97%)	18 (3%)	38	58
1	B	584/666 (88%)	573 (98%)	11 (2%)	50	65
All	All	1236/1332 (93%)	1207 (98%)	29 (2%)	44	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	76	LEU
1	A	177	ASN
1	A	179	THR
1	A	214	GLU
1	A	225	ARG
1	A	346	VAL
1	A	357	LEU
1	A	382	THR
1	A	469	ILE
1	A	491	THR
1	A	513	ILE
1	A	655	ILE
1	A	668	THR
1	A	672	LYS
1	A	681	VAL
1	A	718	ILE

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Mol	Chain	Res	Type
1	A	721	HIS
1	B	15	ASN
1	B	43	GLN
1	B	321	ILE
1	B	357	LEU
1	B	359	LYS
1	B	469	ILE
1	B	534	VAL
1	B	563	MET
1	B	655	ILE
1	B	668	THR
1	B	676	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	219	HIS
1	A	315	ASN
1	A	324	HIS
1	A	453	ASN
1	A	734	GLN
1	A	750	GLN
1	B	71	ASN
1	B	158	GLN
1	B	427	ASN
1	B	447	GLN
1	B	453	ASN
1	B	639	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	PNS	A	801	1	1,4,21	0.95	0	0,4,29	-	-

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	PNS	A	801	1	-	0/0/2/27	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [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	759/776 (97%)	-0.14	6 (0%)	82 62	184, 263, 353, 471	0
1	B	681/776 (87%)	-0.21	6 (0%)	81 60	171, 236, 336, 450	0
All	All	1440/1552 (92%)	-0.17	12 (0%)	82 62	171, 252, 347, 471	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	LEU	3.5
1	B	90	VAL	3.0
1	A	141	PHE	2.6
1	B	113	LEU	2.6
1	B	681	VAL	2.4
1	B	100	ILE	2.4
1	B	278	GLY	2.2
1	B	87	PHE	2.2
1	A	321	ILE	2.2
1	A	573	LEU	2.2
1	A	685	ALA	2.1
1	A	328	SER	2.1

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

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	PNS	A	801	5/22	0.64	0.14	266,268,288,306	0

6.5 Other polymers

There are no such residues in this entry.