



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:49 PM UTC

PDB ID : 9BE3 / pdb_00009be3
Title : The pre-condensation state of the dimodular NRPS protein LgrA
Authors : Pistofidis, A.; Schmeing, T.M.
Deposited on : 2024-04-13
Resolution : 2.90 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

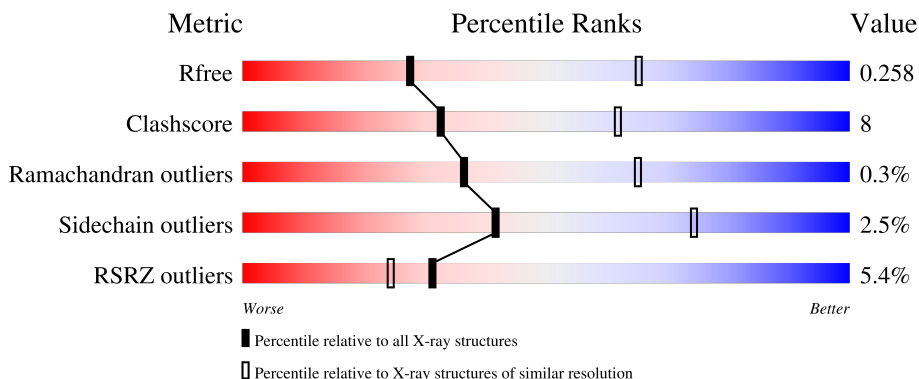
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1814	 4% 76% 21% ..
1	B	1814	 6% 79% 17% ..

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
5	MN	B	1905	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 28355 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 synthase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1774	14120	9015	2413	2634	58	0	1	0
1	B	1746	13627	8719	2307	2544	57	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

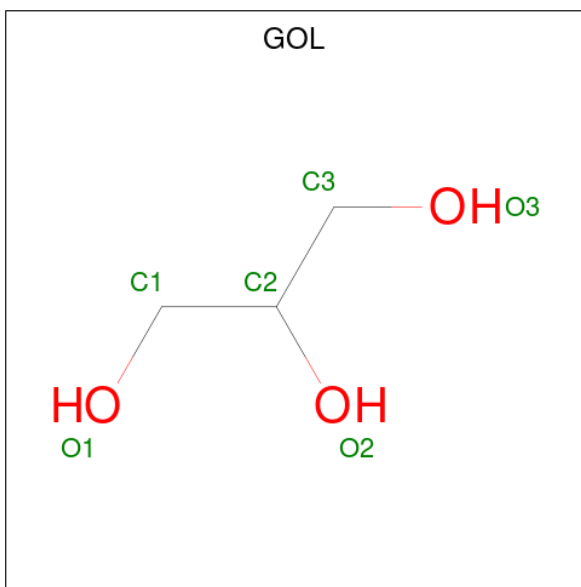
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	770A	ASN	SER	conflict	UNP Q70LM7
A	770B	GLY	-	insertion	UNP Q70LM7
A	771	LEU	-	insertion	UNP Q70LM7
A	1804	ALA	-	expression tag	UNP Q70LM7
A	1805	ALA	-	expression tag	UNP Q70LM7
A	1806	ALA	-	expression tag	UNP Q70LM7
A	1807	GLU	-	expression tag	UNP Q70LM7
A	1808	ASN	-	expression tag	UNP Q70LM7
A	1809	LEU	-	expression tag	UNP Q70LM7
A	1810	TYR	-	expression tag	UNP Q70LM7
A	1811	PHE	-	expression tag	UNP Q70LM7
A	1812	GLN	-	expression tag	UNP Q70LM7
B	1	MET	-	initiating methionine	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	770A	ASN	SER	conflict	UNP Q70LM7
B	770B	GLY	-	insertion	UNP Q70LM7
B	771	LEU	-	insertion	UNP Q70LM7
B	1804	ALA	-	expression tag	UNP Q70LM7
B	1805	ALA	-	expression tag	UNP Q70LM7
B	1806	ALA	-	expression tag	UNP Q70LM7
B	1807	GLU	-	expression tag	UNP Q70LM7
B	1808	ASN	-	expression tag	UNP Q70LM7
B	1809	LEU	-	expression tag	UNP Q70LM7

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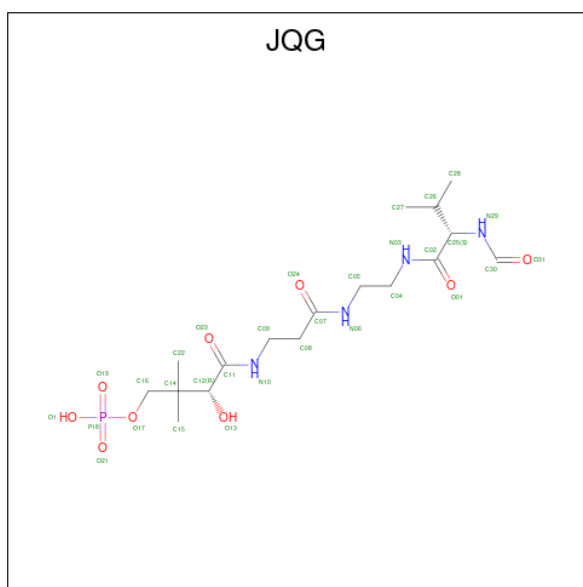
Chain	Residue	Modelled	Actual	Comment	Reference
B	1810	TYR	-	expression tag	UNP Q70LM7
B	1811	PHE	-	expression tag	UNP Q70LM7
B	1812	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



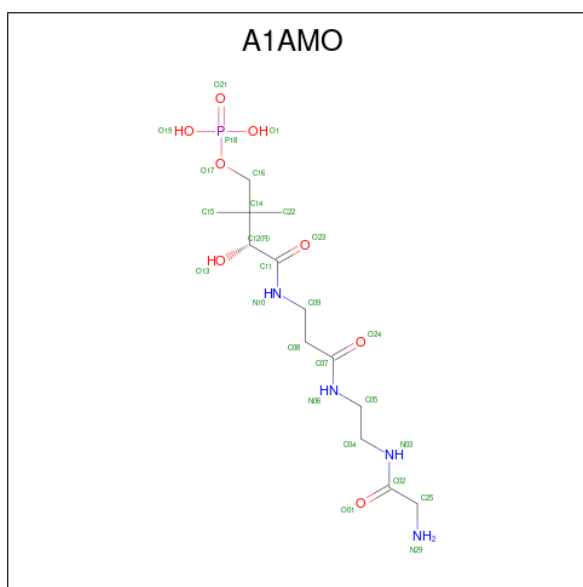
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is (2 {R})- {N}-[3-[2-[(2 {S})-2-formamido-3-methyl-butanoyl]amino]ethylamin o]-3-oxidanylidene-propyl]-3,3-dimethyl-2-oxidanyl-4-[oxidanyl-bis(oxidanylidene)-\$1^{\wedge}\{6\}\$-phosphanyl]oxy-butanamide (CCD ID: JQG) (formula: C₁₇H₃₂N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	30	17	4	8	1	0	0
3	B	1	30	17	4	8	1	0	0

- Molecule 4 is N-[2-(glycylamino)ethyl]-N 3 -(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alaninamide (CCD ID: A1AMO) (formula: $C_{13}H_{27}N_4O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	25	13	4	7	1	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mn 1	0	0
5	B	3	Total 3	Mn 3	0	0

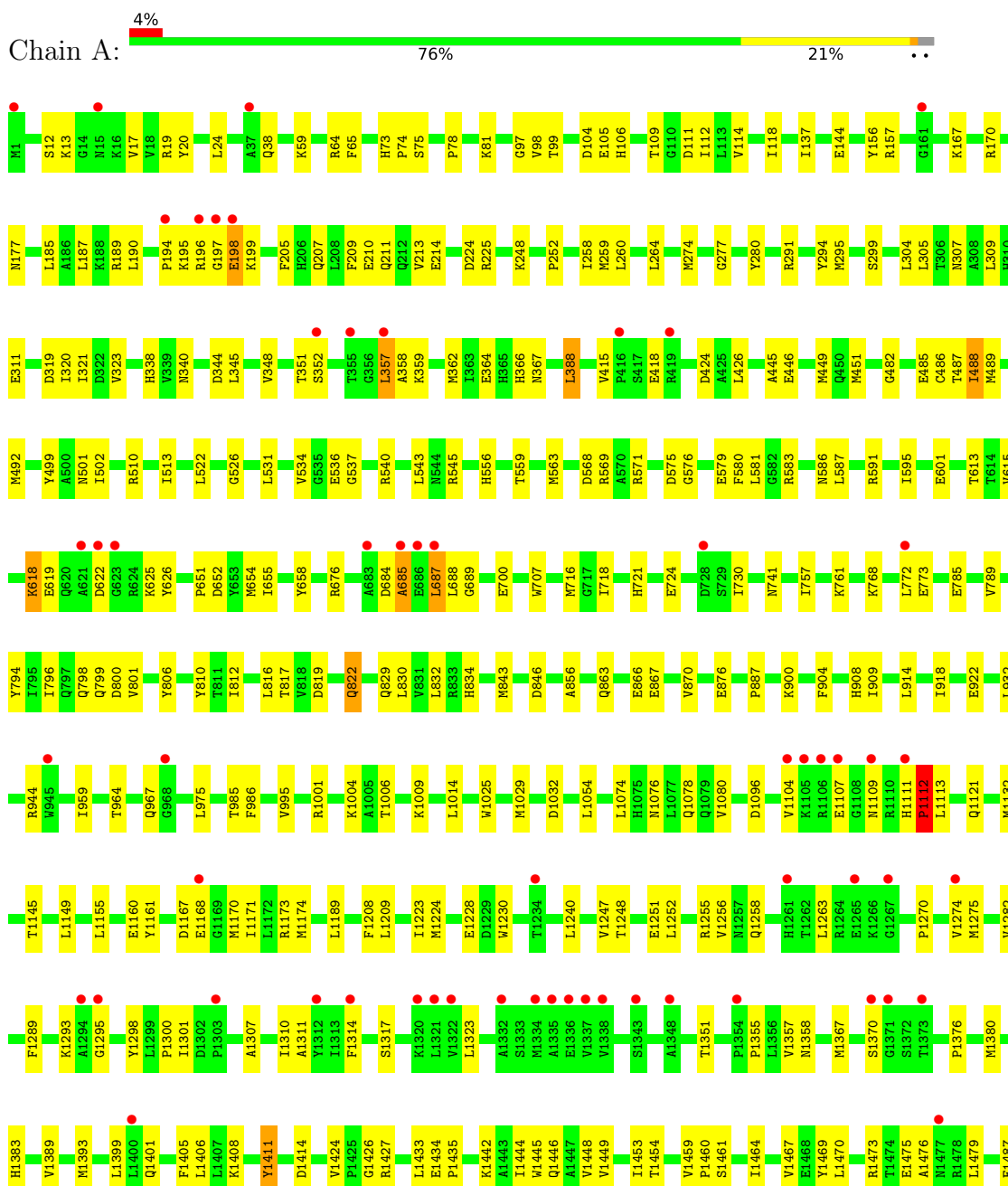
- Molecule 6 is water.

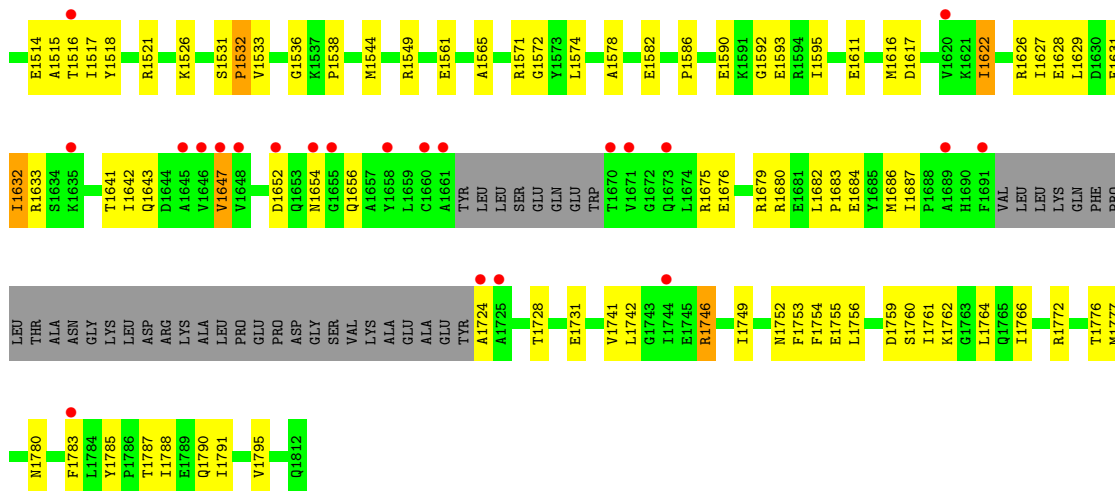
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	277	Total 277	O 277	0	0
6	B	224	Total 224	O 224	0	0

3 Residue-property plots

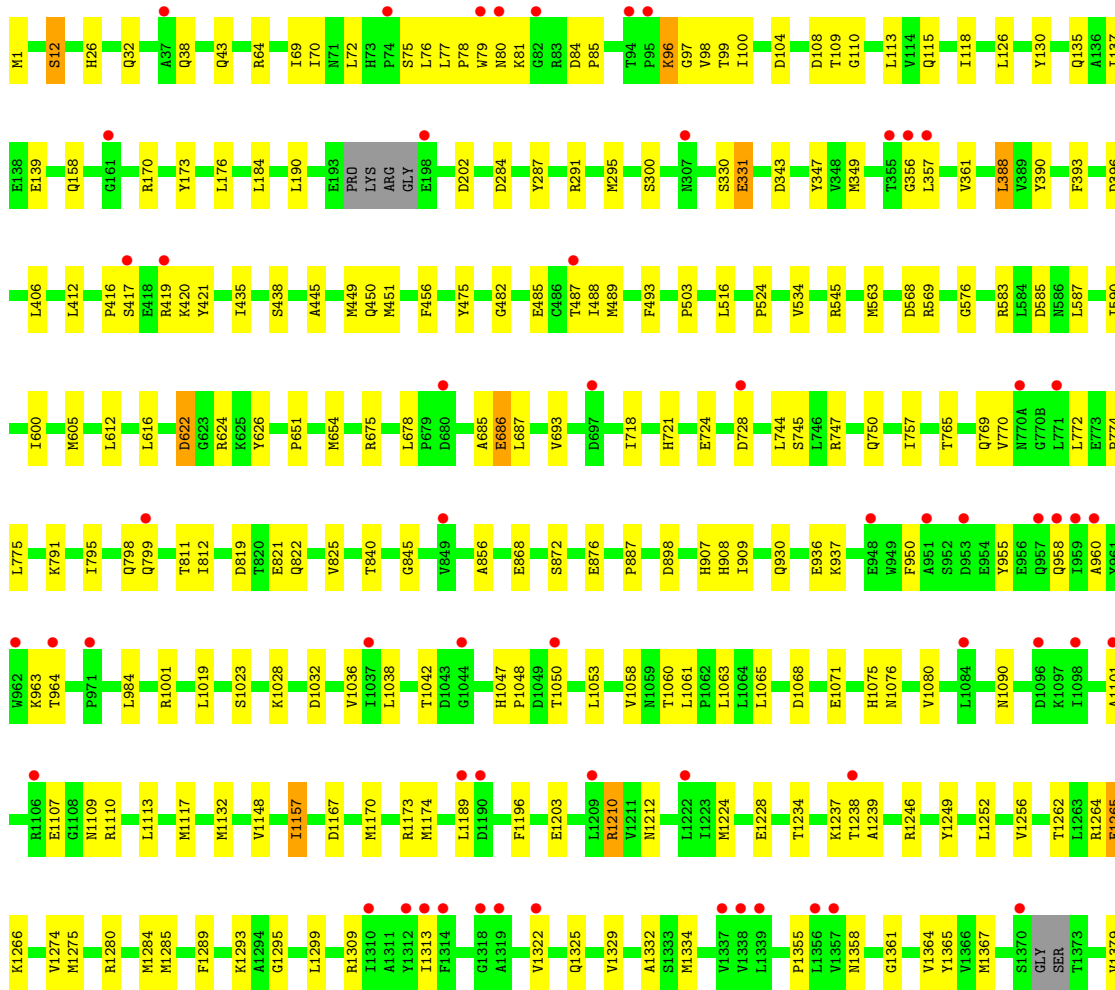
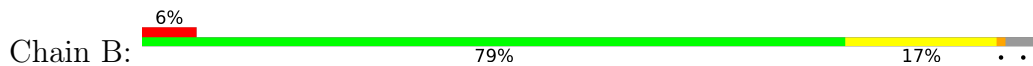
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

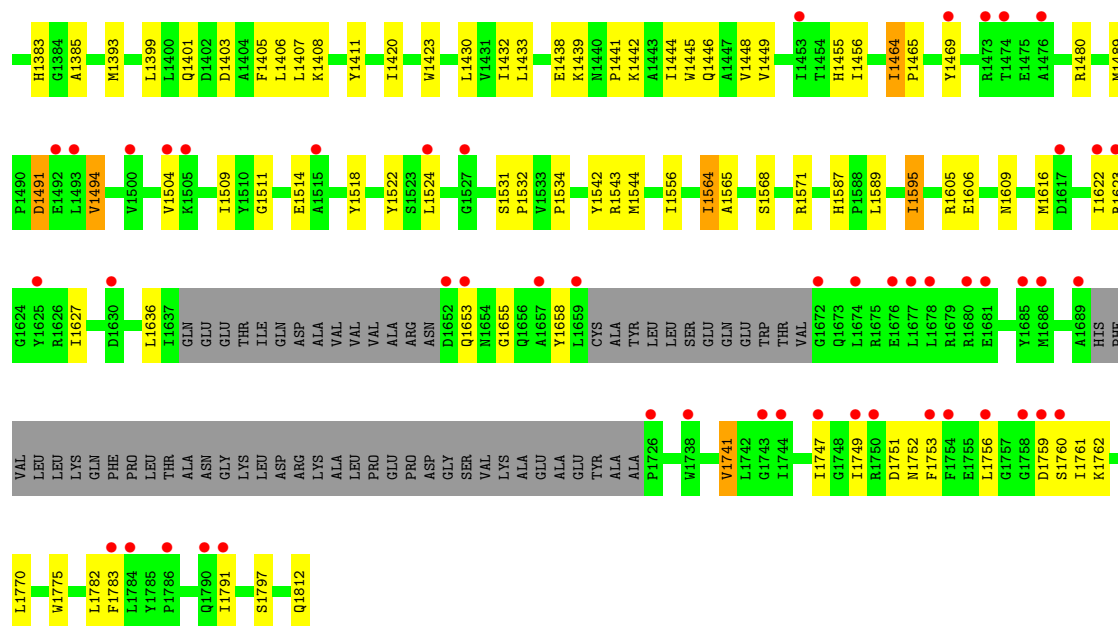
• Molecule 1: Linear gramicidin synthase subunit A





● Molecule 1: Linear gramicidin synthase subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	184.82Å 427.90Å 77.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.90 48.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.74-2.90) 98.9 (48.74-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.216 , 0.258 0.216 , 0.258	Depositor DCC
R_{free} test set	3109 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28355	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JQG, GOL, A1AMO, MN

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	0.16	0/14430	0.33	1/19594 (0.0%)
1	B	0.14	0/13926	0.31	0/18947
All	All	0.15	0/28356	0.32	1/38541 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1643	GLN	N-CA-C	-6.04	106.55	114.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1746	ARG	Sidechain

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	14120	0	14025	252	2
1	B	13627	0	13332	187	2
2	A	12	0	16	0	0
2	B	6	0	8	0	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
4	A	25	0	0	0	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	277	0	0	6	0
6	B	224	0	0	1	0
All	All	28355	0	27381	438	2

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 8.

All (438) 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:248:LYS:NZ	1:A:319:ASP:OD2	2.05	0.88
1:B:130:TYR:OH	1:B:170:ARG:NH2	2.08	0.86
1:B:1759:ASP:OD1	1:B:1760:SER:N	2.09	0.84
1:B:1264:ARG:NH2	1:B:1355:PRO:O	2.11	0.83
1:B:1751:ASP:HB3	1:B:1756:LEU:HD21	1.61	0.82
1:A:1074:LEU:HD21	1:A:1189:LEU:HD23	1.64	0.79
1:A:167:LYS:H	1:A:167:LYS:HD3	1.48	0.79
1:A:1754:PHE:HZ	1:A:1783:PHE:HD1	1.30	0.79
1:A:1307:ALA:HA	1:A:1310:ILE:HG12	1.66	0.76
1:A:170:ARG:NH2	1:A:177:ASN:OD1	2.19	0.76
1:B:291:ARG:HG2	1:B:295:MET:HE2	1.66	0.76
1:A:1590:GLU:HB3	1:A:1593:GLU:HB2	1.68	0.76
1:A:195:LYS:O	1:A:196:ARG:NH1	2.20	0.74
1:B:1050:THR:HA	1:B:1053:LEU:HD23	1.69	0.74
1:A:1684:GLU:HA	1:A:1687:ILE:HD13	1.69	0.74
1:A:619:GLU:HB3	1:A:625:LYS:HE3	1.72	0.71
1:B:605:MET:HE2	1:B:612:LEU:HA	1.71	0.71
1:A:846:ASP:OD1	1:A:1772:ARG:NH2	2.23	0.70
1:A:177:ASN:ND2	1:A:867:GLU:OE1	2.23	0.70
1:B:812:ILE:HG12	1:B:1132:MET:HG2	1.74	0.70
1:A:1258:GLN:HE21	1:A:1351:THR:HG22	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:LEU:HD23	1:A:1408:LYS:HD2	1.75	0.69
1:A:1107:GLU:OE2	1:A:1684:GLU:N	2.27	0.68
1:B:747:ARG:HB2	1:B:750:GLN:HG3	1.76	0.68
1:A:1025:TRP:HZ2	1:A:1174:MET:HB3	1.59	0.68
1:B:388:LEU:HD13	1:B:435:ILE:HG21	1.77	0.67
1:B:1565:ALA:HB2	1:B:1595:ILE:HG22	1.76	0.67
1:B:1210:ARG:NH2	1:B:1606:GLU:O	2.28	0.67
1:A:277:GLY:HA2	1:A:340:ASN:HD21	1.59	0.66
1:A:1228:GLU:OE1	1:A:1293:LYS:NZ	2.28	0.66
1:A:59:LYS:HG3	1:A:105:GLU:HG2	1.77	0.66
1:B:1023:SER:HB3	1:B:1036:VAL:HG21	1.78	0.66
1:A:13:LYS:HD3	1:A:13:LYS:N	2.10	0.66
1:A:345:LEU:HD11	1:A:362:MET:HE3	1.77	0.66
1:B:81:LYS:HB3	1:B:108:ASP:HB2	1.79	0.65
1:A:591:ARG:HH21	1:A:652:ASP:HB3	1.60	0.65
1:A:1633:ARG:HB2	1:A:1647:VAL:HG21	1.79	0.65
1:A:1627:ILE:HG23	1:A:1686:MET:HG2	1.78	0.65
1:A:205:PHE:HD2	1:A:274:MET:HE1	1.61	0.64
1:B:1464:ILE:HG23	1:B:1465:PRO:HD3	1.79	0.63
1:A:258:ILE:HD12	1:A:280:TYR:HB2	1.79	0.62
1:B:622:ASP:OD1	1:B:624:ARG:NH1	2.32	0.62
1:A:1401:GLN:OE1	1:A:1427:ARG:NH2	2.32	0.62
1:A:367:ASN:ND2	1:A:536:GLU:O	2.31	0.62
1:B:1441:PRO:HG2	1:B:1469:TYR:CD2	2.34	0.62
1:A:367:ASN:HB3	1:A:487:THR:OG1	1.98	0.62
1:A:1263:LEU:HD21	1:A:1323:LEU:HD11	1.82	0.62
1:B:420:LYS:HE2	1:B:421:TYR:HE1	1.64	0.61
1:A:922:GLU:HG2	1:A:932:LEU:HD13	1.80	0.61
1:B:1405:PHE:HD1	1:B:1406:LEU:H	1.49	0.61
1:A:1632:ILE:HA	1:A:1682:LEU:HD21	1.83	0.61
1:A:1777:MET:HG3	1:A:1795:VAL:HG12	1.82	0.61
1:B:693:VAL:HB	1:B:718:ILE:HG12	1.83	0.61
1:A:1252:LEU:O	1:A:1256:VAL:HG23	2.00	0.61
1:A:1310:ILE:HG13	1:A:1311:ALA:N	2.16	0.61
1:B:104:ASP:OD2	1:B:109:THR:OG1	2.18	0.61
1:A:1004:LYS:HD3	1:A:1014:LEU:HD22	1.83	0.60
1:B:1494:VAL:HB	1:B:1524:LEU:HD23	1.82	0.60
1:A:569:ARG:HG2	1:A:581:LEU:HB2	1.83	0.60
1:B:488:ILE:HG22	1:B:489:MET:HG3	1.83	0.60
1:B:622:ASP:OD1	1:B:624:ARG:HG3	2.02	0.60
1:B:1238:THR:HG21	1:B:1246:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:GLU:HG2	1:B:1075:HIS:ND1	2.18	0.59
1:A:73:HIS:CD2	1:A:75:SER:HB3	2.37	0.59
1:A:104:ASP:OD1	1:A:106:HIS:N	2.36	0.59
1:B:960:ALA:O	1:B:964:THR:HG22	2.02	0.59
1:A:1531:SER:OG	1:A:1532:PRO:HD3	2.03	0.58
1:A:526:GLY:HA2	1:A:571:ARG:HD3	1.84	0.58
1:A:1275:MET:HE1	1:A:1314:PHE:CD1	2.38	0.58
1:A:571:ARG:NH2	6:A:2003:HOH:O	2.35	0.58
1:A:1006:THR:HG23	1:A:1189:LEU:HD21	1.86	0.58
1:A:1461:SER:HA	1:A:1464:ILE:HD12	1.85	0.58
1:B:963:LYS:HG3	1:B:1101:ALA:HB1	1.86	0.58
1:A:1785:TYR:HB3	1:A:1790:GLN:HB3	1.84	0.58
1:A:1298:TYR:CE2	1:A:1300:PRO:HG3	2.39	0.58
1:B:1047:HIS:CD2	1:B:1048:PRO:HD2	2.39	0.57
1:A:1445:TRP:O	1:A:1449:VAL:HG23	2.05	0.57
1:A:687:LEU:C	1:A:689:GLY:H	2.12	0.57
1:A:1405:PHE:HD1	1:A:1406:LEU:H	1.52	0.57
1:B:1393:MET:HE1	1:B:1509:ILE:HD13	1.86	0.57
1:B:173:TYR:HB3	1:B:176:LEU:HD12	1.86	0.57
1:A:768:LYS:NZ	6:A:2004:HOH:O	2.38	0.56
1:A:799:GLN:HG3	1:A:800:ASP:N	2.18	0.56
1:B:1076:ASN:O	1:B:1080:VAL:HG23	2.05	0.56
1:B:1285:MET:HE1	1:B:1420:ILE:HA	1.85	0.56
1:B:1322:VAL:HG11	1:B:1332:ALA:HB1	1.87	0.56
1:B:98:VAL:HB	1:B:137:ILE:HD13	1.87	0.56
1:A:569:ARG:NH2	1:A:587:LEU:HD11	2.20	0.56
1:B:1063:LEU:HB3	1:B:1065:LEU:HD11	1.87	0.56
1:B:1262:THR:O	1:B:1266:LYS:HG2	2.05	0.56
1:B:1393:MET:HE2	1:B:1518:TYR:CD2	2.41	0.56
1:A:485:GLU:OE1	1:A:485:GLU:N	2.38	0.56
1:B:772:LEU:O	1:B:774:PRO:HD3	2.06	0.56
1:A:260:LEU:HD11	1:A:323:VAL:HG11	1.86	0.56
1:A:1626:ARG:HH22	1:A:1628:GLU:CD	2.13	0.56
1:B:202:ASP:N	1:B:202:ASP:OD1	2.39	0.56
1:B:721:HIS:HB3	1:B:724:GLU:HB2	1.88	0.55
1:B:347:TYR:CE1	1:B:349:MET:HE2	2.41	0.55
1:A:167:LYS:H	1:A:167:LYS:CD	2.18	0.55
1:A:718:ILE:HA	1:A:757:ILE:HB	1.88	0.55
1:B:420:LYS:HG3	1:B:421:TYR:CE1	2.42	0.55
1:B:950:PHE:O	1:B:955:TYR:HD2	1.89	0.55
1:A:114:VAL:HG21	1:A:144:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:GLU:OE2	1:B:937:LYS:HG2	2.06	0.55
1:B:1109:ASN:OD1	1:B:1110:ARG:HG3	2.05	0.55
1:A:1367:MET:HE3	1:A:1414:ASP:HA	1.88	0.55
1:A:975:LEU:HD22	1:A:1029:MET:HE3	1.89	0.54
1:A:1355:PRO:HG3	1:B:1265:GLU:HA	1.89	0.54
1:A:1389:VAL:HG21	1:A:1516:THR:OG1	2.06	0.54
1:A:1469:TYR:HD1	1:A:1470:LEU:HD12	1.72	0.54
1:B:1228:GLU:OE2	1:B:1293:LYS:NZ	2.32	0.54
1:A:534:VAL:HG22	1:A:563:MET:HG2	1.88	0.54
1:A:190:LEU:HD21	1:A:576:GLY:HA2	1.89	0.54
1:A:1749:ILE:HA	1:A:1788:ILE:HB	1.88	0.54
1:A:676:ARG:HA	1:A:676:ARG:NE	2.22	0.54
1:B:821:GLU:O	1:B:825:VAL:HG23	2.08	0.54
1:B:744:LEU:HD23	1:B:770:VAL:HA	1.90	0.54
1:B:1491:ASP:OD1	1:B:1491:ASP:N	2.40	0.54
1:A:388:LEU:HD21	1:A:426:LEU:HD11	1.89	0.54
1:A:98:VAL:HB	1:A:137:ILE:HD13	1.88	0.54
1:B:791:LYS:O	1:B:795:ILE:HG13	2.07	0.54
1:A:1167:ASP:OD1	1:A:1170:MET:HG3	2.08	0.53
1:A:1521:ARG:O	1:A:1536:GLY:HA3	2.08	0.53
1:A:1442:LYS:O	1:A:1446:GLN:HG3	2.09	0.53
1:B:1060:THR:HG22	1:B:1117:MET:HE1	1.90	0.53
1:A:816:LEU:HD23	1:A:900:LYS:HG3	1.88	0.53
1:B:685:ALA:O	1:B:686:GLU:HB2	2.08	0.53
1:A:1683:PRO:HD2	1:A:1686:MET:HE2	1.90	0.53
1:B:419:ARG:HD2	1:B:419:ARG:O	2.09	0.53
1:A:224:ASP:OD1	1:A:225:ARG:NH1	2.43	0.52
1:A:914:LEU:O	1:A:918:ILE:HG13	2.08	0.52
1:B:856:ALA:HB1	1:B:887:PRO:HD3	1.91	0.52
1:A:856:ALA:HB1	1:A:887:PRO:HD3	1.91	0.52
1:B:1:MET:HG2	1:B:26:HIS:CE1	2.44	0.52
1:A:834:HIS:CG	1:A:1054:LEU:HD22	2.45	0.52
1:B:568:ASP:OD1	1:B:583:ARG:NH1	2.40	0.52
1:B:1379:VAL:HG11	1:B:1514:GLU:HA	1.92	0.52
1:A:1675:ARG:O	1:A:1679:ARG:N	2.43	0.52
1:A:1780:ASN:HA	1:A:1783:PHE:CE2	2.44	0.52
1:B:1752:ASN:O	1:B:1756:LEU:HG	2.09	0.52
1:A:99:THR:HG23	1:A:112:ILE:HG23	1.91	0.52
1:B:516:LEU:HD11	1:B:563:MET:HE1	1.92	0.52
1:B:1531:SER:OG	1:B:1532:PRO:HD3	2.10	0.52
1:A:291:ARG:NH1	1:A:295:MET:HE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:HA	1:A:451:MET:HE2	1.92	0.51
1:B:1001:ARG:HG2	1:B:1001:ARG:HH11	1.73	0.51
1:B:1442:LYS:O	1:B:1446:GLN:HG3	2.09	0.51
1:A:1622:ILE:HB	1:A:1627:ILE:HD11	1.93	0.51
1:A:1676:GLU:HA	1:A:1679:ARG:HB2	1.92	0.51
1:B:898:ASP:OD1	1:B:898:ASP:N	2.43	0.51
1:B:1107:GLU:OE2	1:B:1623:ARG:NH1	2.44	0.51
1:A:97:GLY:HA2	1:A:118:ILE:H	1.76	0.51
1:A:568:ASP:HB3	1:A:580:PHE:HE1	1.75	0.51
1:A:964:THR:O	1:A:967:GLN:HG2	2.11	0.51
1:A:207:GLN:HG2	1:A:338:HIS:CE1	2.46	0.51
1:A:556:HIS:HB2	1:A:563:MET:HE3	1.93	0.51
1:A:1104:VAL:HG21	1:A:1113:LEU:HG	1.92	0.51
1:A:513:ILE:HD12	1:A:531:LEU:HD21	1.92	0.51
1:B:1812:GLN:NE2	6:B:2001:HOH:O	2.41	0.51
1:A:111:ASP:OD2	1:A:157:ARG:HG2	2.11	0.50
1:B:99:THR:HG23	1:B:115:GLN:HG3	1.92	0.50
1:A:259:MET:HE2	1:A:304:LEU:HD21	1.93	0.50
1:A:1654:ASN:C	1:A:1656:GLN:H	2.19	0.50
1:A:1270:PRO:HG3	1:A:1357:VAL:O	2.11	0.50
1:A:1679:ARG:NH1	1:A:1755:GLU:OE2	2.45	0.50
1:B:170:ARG:O	1:B:170:ARG:HG2	2.11	0.50
1:B:1063:LEU:HB3	1:B:1065:LEU:CD1	2.41	0.50
1:B:1170:MET:O	1:B:1174:MET:HG3	2.12	0.50
1:B:1544:MET:HG2	1:B:1564:ILE:HG23	1.94	0.50
1:A:185:LEU:O	1:A:189:ARG:HG3	2.11	0.50
1:A:311:GLU:HG3	1:A:320:ILE:HG21	1.92	0.50
1:A:571:ARG:NH1	1:A:579:GLU:OE2	2.45	0.50
1:A:721:HIS:HB3	1:A:724:GLU:HB2	1.94	0.50
1:A:794:TYR:O	1:A:798:GLN:HG2	2.12	0.50
1:A:1240:LEU:HD12	1:A:1282:VAL:HG13	1.93	0.50
1:A:1310:ILE:HG13	1:A:1311:ALA:H	1.77	0.50
1:B:1408:LYS:HD3	1:B:1456:ILE:HD11	1.93	0.50
1:A:1109:ASN:ND2	1:A:1683:PRO:HB3	2.27	0.50
1:B:76:LEU:HD13	1:B:97:GLY:HA3	1.93	0.50
1:B:445:ALA:O	1:B:449:MET:HG3	2.12	0.50
1:A:812:ILE:HG12	1:A:1132:MET:HG2	1.93	0.50
1:B:1522:TYR:CE2	1:B:1534:PRO:HD2	2.46	0.50
1:A:224:ASP:HB3	1:A:264:LEU:HG	1.93	0.49
1:A:830:LEU:HD21	1:A:922:GLU:HB3	1.94	0.49
1:A:482:GLY:HA3	1:A:489:MET:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD21	1:A:522:LEU:HG	1.94	0.49
1:A:305:LEU:HD23	1:A:321:ILE:HB	1.94	0.49
1:B:97:GLY:HA2	1:B:118:ILE:HG23	1.93	0.49
1:A:1626:ARG:HG2	1:A:1626:ARG:HH11	1.77	0.49
1:A:843:MET:HE1	1:A:1764:LEU:HG	1.95	0.49
1:B:1445:TRP:O	1:B:1449:VAL:HG23	2.13	0.49
1:B:626:TYR:HB3	1:B:687:LEU:HD13	1.95	0.49
1:A:207:GLN:O	1:A:211:GLN:HG3	2.13	0.49
1:A:1111[A]:HIS:CD2	1:A:1112:PRO:HD2	2.47	0.48
1:A:1224:MET:HE1	1:A:1383:HIS:NE2	2.28	0.48
1:B:1256:VAL:HG11	1:B:1289:PHE:HB3	1.95	0.48
1:A:1107:GLU:HG3	1:A:1684:GLU:HB2	1.93	0.48
1:B:1173:ARG:HD2	1:B:1203:GLU:OE2	2.12	0.48
1:A:78:PRO:O	1:A:81:LYS:HD2	2.13	0.48
1:B:84:ASP:OD1	1:B:170:ARG:NH1	2.34	0.48
1:A:1752:ASN:HB3	1:A:1755:GLU:HG3	1.95	0.48
1:B:1334:MET:HE3	1:B:1334:MET:HA	1.96	0.48
1:A:601:GLU:HG2	1:A:615:VAL:HG23	1.94	0.48
1:B:190:LEU:HD21	1:B:576:GLY:HA2	1.94	0.48
1:A:12:SER:OG	1:A:13:LYS:N	2.47	0.48
1:B:291:ARG:O	1:B:295:MET:HG3	2.13	0.48
1:B:1252:LEU:O	1:B:1256:VAL:HG23	2.14	0.48
1:A:291:ARG:HH11	1:A:295:MET:HE2	1.79	0.48
1:A:1449:VAL:HG13	1:A:1476:ALA:O	2.14	0.48
1:B:135:GLN:O	1:B:139:GLU:HG2	2.13	0.48
1:B:1028:LYS:NZ	1:B:1196:PHE:O	2.47	0.48
1:A:1752:ASN:O	1:A:1756:LEU:HG	2.13	0.48
1:B:1309:ARG:O	1:B:1313:ILE:HG13	2.14	0.48
1:B:1361:GLY:O	1:B:1571:ARG:NH2	2.46	0.48
1:B:70:ILE:HD12	1:B:113:LEU:HD11	1.96	0.47
1:A:556:HIS:ND1	1:A:559:THR:HG23	2.30	0.47
1:B:284:ASP:HB3	1:B:287:TYR:CD2	2.49	0.47
1:B:1042:THR:O	1:B:1058:VAL:HA	2.14	0.47
1:B:1511:GLY:HA3	1:B:1518:TYR:HA	1.95	0.47
1:A:785:GLU:OE1	1:A:944:ARG:NE	2.47	0.47
1:A:1754:PHE:HZ	1:A:1783:PHE:CD1	2.20	0.47
1:A:601:GLU:HB3	1:A:613:THR:HG23	1.96	0.47
1:A:1728:THR:CG2	1:A:1731:GLU:HG3	2.44	0.47
1:A:618:LYS:NZ	1:A:676:ARG:HH22	2.13	0.47
1:A:1230:TRP:CE3	1:A:1427:ARG:HD3	2.49	0.47
1:A:1298:TYR:HE2	1:A:1300:PRO:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:ASP:H	1:A:1762:LYS:HG3	1.80	0.47
1:B:1075:HIS:C	1:B:1075:HIS:CD2	2.93	0.47
1:B:1587:HIS:CE1	1:B:1589:LEU:HD12	2.50	0.47
1:B:1753:PHE:HA	1:B:1756:LEU:HD12	1.97	0.47
1:A:1009:LYS:HA	1:A:1009:LYS:HD2	1.70	0.47
1:A:1565:ALA:HB2	1:A:1595:ILE:HG22	1.97	0.47
1:A:1460:PRO:HB2	1:A:1487:GLU:HG3	1.96	0.47
1:B:126:LEU:HD21	1:B:184:LEU:HD22	1.95	0.47
1:B:417:SER:HA	1:B:420:LYS:HG2	1.96	0.47
1:A:196:ARG:NH1	1:A:197:GLY:O	2.48	0.47
1:B:485:GLU:OE1	1:B:485:GLU:N	2.45	0.47
1:B:1542:TYR:CZ	1:B:1568:SER:HB2	2.50	0.47
1:B:390:TYR:CE1	1:B:420:LYS:HB2	2.50	0.46
1:B:416:PRO:HD2	1:B:419:ARG:NH1	2.31	0.46
1:A:351:THR:HG23	1:A:359:LYS:HE3	1.97	0.46
1:A:575:ASP:OD1	1:A:575:ASP:N	2.48	0.46
1:A:487:THR:O	1:A:489:MET:N	2.49	0.46
1:A:1317:SER:HA	1:A:1574:LEU:HD21	1.97	0.46
1:B:493:PHE:CE2	1:B:503:PRO:HD2	2.49	0.46
1:B:1280:ARG:HG2	1:B:1432:ILE:HG23	1.97	0.46
1:B:1399:LEU:HD12	1:B:1455:HIS:CG	2.51	0.46
1:B:77:LEU:HA	1:B:79:TRP:H	1.79	0.46
1:B:600:ILE:HD13	1:B:654:MET:O	2.15	0.46
1:A:446:GLU:HA	1:A:449:MET:HE3	1.98	0.46
1:A:1515:ALA:O	1:A:1516:THR:OG1	2.34	0.46
1:A:1742:LEU:HD13	1:A:1756:LEU:HB2	1.97	0.46
1:B:1068:ASP:OD2	1:B:1071:GLU:HB2	2.16	0.46
1:B:1655:GLY:HA3	1:B:1658:TYR:O	2.16	0.46
1:A:1434:GLU:HG3	1:A:1435:PRO:HD2	1.98	0.45
1:B:487:THR:HG22	1:B:488:ILE:HD12	1.98	0.45
1:B:1148:VAL:HG22	1:B:1157:ILE:HD13	1.99	0.45
1:A:1454:THR:HA	1:A:1479:LEU:HA	1.98	0.45
1:A:1442:LYS:HG3	1:A:1469:TYR:CZ	2.52	0.45
1:A:1753:PHE:HZ	1:A:1762:LYS:HB2	1.81	0.45
1:B:872:SER:O	1:B:876:GLU:HG3	2.15	0.45
1:B:1036:VAL:HG23	1:B:1065:LEU:HB2	1.98	0.45
1:B:1556:ILE:HD13	1:B:1606:GLU:HA	1.98	0.45
1:A:252:PRO:HB3	1:A:344:ASP:OD2	2.16	0.45
1:A:1652:ASP:N	1:A:1656:GLN:O	2.38	0.45
1:A:1514:GLU:OE1	1:A:1514:GLU:N	2.41	0.45
1:A:1173:ARG:NH1	6:A:2009:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:ILE:O	1:A:1448:VAL:HG23	2.17	0.45
1:A:1076:ASN:O	1:A:1080:VAL:HG23	2.17	0.45
1:B:356:GLY:C	1:B:357:LEU:HD23	2.41	0.45
1:B:420:LYS:HG3	1:B:421:TYR:CD1	2.52	0.45
1:B:569:ARG:NH2	1:B:587:LEU:HD13	2.32	0.45
1:B:1444:ILE:O	1:B:1448:VAL:HG23	2.17	0.45
1:A:366:HIS:ND1	1:A:536:GLU:OE1	2.46	0.45
1:B:77:LEU:HA	1:B:77:LEU:HD23	1.80	0.45
1:B:96:LYS:H	1:B:96:LYS:HG2	1.60	0.45
1:A:501:ASN:ND2	6:A:2008:HOH:O	2.49	0.45
1:B:77:LEU:HD22	1:B:78:PRO:HA	1.99	0.45
1:B:799:GLN:HG3	1:B:1783:PHE:CE1	2.52	0.45
1:A:1301:ILE:O	1:A:1411:TYR:OH	2.30	0.44
1:A:1393:MET:HE2	1:A:1518:TYR:CD2	2.53	0.44
1:A:1170:MET:HE2	1:A:1170:MET:HB3	1.76	0.44
1:A:1224:MET:HE2	1:A:1224:MET:HB3	1.87	0.44
1:A:1777:MET:HE2	1:A:1791:ILE:HD13	1.98	0.44
1:B:1113:LEU:HD23	1:B:1113:LEU:HA	1.77	0.44
1:B:1393:MET:HE1	1:B:1509:ILE:CD1	2.47	0.44
1:A:348:VAL:HG22	1:A:362:MET:HG2	1.99	0.44
1:A:299:SER:HA	1:A:543:LEU:HD21	2.00	0.44
1:A:362:MET:CE	1:A:540:ARG:HD2	2.48	0.44
1:A:1121:GLN:HB2	1:A:1149:LEU:HD23	1.99	0.44
1:A:1240:LEU:HB2	1:A:1247:VAL:HB	2.00	0.44
1:A:591:ARG:NH2	1:A:652:ASP:HB3	2.30	0.44
1:A:1549:ARG:NH2	6:A:2006:HOH:O	2.47	0.44
1:A:1096:ASP:OD1	1:A:1096:ASP:N	2.48	0.44
1:B:349:MET:O	1:B:361:VAL:N	2.49	0.44
1:A:19:ARG:NH1	1:A:876:GLU:OE2	2.46	0.44
1:A:205:PHE:CD2	1:A:274:MET:HE1	2.45	0.44
1:A:654:MET:HE2	1:A:654:MET:HB3	1.89	0.44
1:A:995:VAL:HB	1:A:1155:LEU:HB2	1.99	0.44
1:A:1538:PRO:HB3	1:A:1544:MET:HG3	2.00	0.44
1:B:72:LEU:HG	1:B:100:ILE:HD13	2.00	0.44
1:B:745:SER:O	1:B:769:GLN:NE2	2.51	0.44
1:B:1399:LEU:HD22	1:B:1423:TRP:HA	1.98	0.44
1:A:352:SER:OG	1:A:357:LEU:O	2.30	0.44
1:A:819:ASP:HB3	1:A:822:GLN:HB2	2.00	0.44
1:B:12:SER:OG	1:B:876:GLU:OE1	2.30	0.44
1:B:1239:ALA:HB2	1:B:1249:TYR:CD1	2.52	0.44
1:B:1393:MET:HE2	1:B:1518:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1605:ARG:HH21	1:B:1609:ASN:HD22	1.64	0.44
1:A:1248:THR:CG2	1:A:1251:GLU:H	2.31	0.43
1:B:616:LEU:HD21	1:B:675:ARG:HD2	2.00	0.43
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.81	0.43
1:B:1364:VAL:HG13	1:B:1365:TYR:CD2	2.53	0.43
1:A:364:GLU:OE1	1:A:366:HIS:NE2	2.51	0.43
1:B:775:LEU:HB3	1:B:937:LYS:HE3	2.00	0.43
1:A:1380:MET:CE	1:A:1571:ARG:HD2	2.48	0.43
1:B:75:SER:HB3	1:B:85:PRO:HB2	2.01	0.43
1:B:795:ILE:HD13	1:B:1761:ILE:HB	2.00	0.43
1:B:406:LEU:HG	1:B:412:LEU:HD11	1.99	0.43
1:B:1622:ILE:HB	1:B:1627:ILE:HD11	2.00	0.43
1:A:1464:ILE:HA	1:A:1467:VAL:HG22	1.99	0.43
1:B:1403:ASP:OD1	1:B:1480:ARG:NH2	2.51	0.43
1:A:20:TYR:CZ	1:A:24:LEU:HD11	2.53	0.43
1:A:64:ARG:HG2	1:A:65:PHE:CE1	2.54	0.43
1:A:829:GLN:O	1:A:832:LEU:HD12	2.18	0.43
1:B:1224:MET:H	1:B:1224:MET:HG2	1.56	0.43
1:A:1406:LEU:HD11	1:A:1433:LEU:HD13	2.00	0.43
1:A:1473:ARG:HG3	1:A:1475:GLU:OE1	2.18	0.43
1:B:482:GLY:HA3	1:B:489:MET:HA	2.00	0.43
1:B:1212:ASN:HB3	1:B:1543:ARG:HG2	2.00	0.43
1:A:388:LEU:HG	1:A:415:VAL:CG2	2.49	0.43
1:A:1074:LEU:O	1:A:1078:GLN:HG2	2.19	0.43
1:A:1145:THR:HB	1:A:1160:GLU:HB3	2.00	0.43
1:B:1406:LEU:HD11	1:B:1433:LEU:HD13	2.01	0.43
1:A:307:ASN:OD1	1:A:309:LEU:N	2.51	0.43
1:A:1728:THR:HG23	1:A:1731:GLU:HG3	2.00	0.43
1:B:85:PRO:HD2	1:B:868:GLU:OE1	2.18	0.43
1:B:176:LEU:HD23	1:B:524:PRO:HG3	2.01	0.43
1:B:718:ILE:HA	1:B:757:ILE:HB	2.01	0.43
1:B:1224:MET:HE2	1:B:1383:HIS:NE2	2.34	0.43
1:B:1367:MET:HE2	1:B:1367:MET:HB2	1.80	0.43
1:A:445:ALA:O	1:A:449:MET:HG3	2.19	0.43
1:A:1295:GLY:HA2	1:A:1358:ASN:OD1	2.18	0.43
1:A:1380:MET:HE3	1:A:1571:ARG:HD2	2.01	0.43
1:B:1770:LEU:HB3	1:B:1775:TRP:HB2	2.01	0.43
1:A:618:LYS:HZ1	1:A:676:ARG:HH22	1.67	0.42
1:A:1256:VAL:HG11	1:A:1289:PHE:HB3	2.00	0.42
1:B:287:TYR:CD2	1:B:295:MET:HE1	2.54	0.42
1:B:349:MET:HE3	1:B:396:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1438:GLU:HG2	1:B:1439:LYS:HG3	2.00	0.42
1:A:112:ILE:HB	1:A:156:TYR:CE1	2.55	0.42
1:A:1161:TYR:CG	1:A:1171:ILE:HG13	2.54	0.42
1:B:624:ARG:HG3	1:B:624:ARG:HH11	1.84	0.42
1:A:210:GLU:O	1:A:214:GLU:HG2	2.19	0.42
1:A:1223:ILE:HD11	1:A:1424:VAL:HB	2.01	0.42
1:A:1399:LEU:O	1:A:1426:GLY:HA3	2.19	0.42
1:A:1442:LYS:HG3	1:A:1469:TYR:CE2	2.54	0.42
1:B:1:MET:HE2	1:B:1:MET:HB2	1.90	0.42
1:A:1459:VAL:HG22	1:A:1460:PRO:O	2.19	0.42
1:B:69:ILE:C	1:B:70:ILE:HD13	2.45	0.42
1:A:1032:ASP:HB2	1:A:1549:ARG:HD3	2.02	0.42
1:A:1230:TRP:CE3	1:A:1230:TRP:HA	2.55	0.42
1:A:1380:MET:HG3	1:A:1572:GLY:O	2.19	0.42
1:B:78:PRO:HB3	1:B:158:GLN:OE1	2.19	0.42
1:B:110:GLY:O	1:B:158:GLN:NE2	2.53	0.42
1:B:1407:LEU:HB2	1:B:1430:LEU:HD11	1.99	0.42
1:A:106:HIS:HB2	1:A:109:THR:OG1	2.20	0.42
1:A:488:ILE:HG22	1:A:489:MET:HG3	2.02	0.42
1:A:618:LYS:HB2	1:A:626:TYR:CE1	2.55	0.42
1:A:13:LYS:NZ	1:A:863:GLN:OE1	2.53	0.42
1:A:684:ASP:O	1:A:685:ALA:C	2.63	0.42
1:A:1113:LEU:HD23	1:A:1113:LEU:HA	1.87	0.42
1:A:1370:SER:O	1:A:1370:SER:OG	2.32	0.42
1:B:331:GLU:CD	1:B:331:GLU:H	2.27	0.42
1:B:585:ASP:C	1:B:585:ASP:OD1	2.63	0.42
1:A:486:CYS:HA	1:A:537:GLY:O	2.19	0.42
1:A:489:MET:SD	1:A:492:MET:HE1	2.60	0.42
1:A:866:GLU:O	1:A:870:VAL:HG23	2.20	0.42
1:A:1370:SER:H	1:A:1376:PRO:HA	1.85	0.42
1:A:1586:PRO:HB3	1:A:1592:GLY:O	2.19	0.42
1:B:907:HIS:HB3	1:B:909:ILE:HG22	2.01	0.42
1:B:1019:LEU:HD11	1:B:1038:LEU:HD11	2.02	0.42
1:B:1167:ASP:CG	1:B:1170:MET:HG3	2.45	0.42
1:B:1275:MET:HA	1:B:1299:LEU:HB3	2.02	0.42
1:B:1295:GLY:HA2	1:B:1358:ASN:OD1	2.20	0.42
1:A:741:ASN:OD1	1:A:772:LEU:HD13	2.20	0.41
1:A:1741:VAL:HG21	1:A:1766:ILE:HG13	2.02	0.41
1:B:651:PRO:HG2	1:B:654:MET:HG3	2.01	0.41
1:B:1385:ALA:HA	1:B:1568:SER:HA	2.02	0.41
1:A:198:GLU:HB2	1:A:199:LYS:H	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ARG:HB2	1:A:586:ASN:HB2	2.02	0.41
1:A:1111[A]:HIS:CG	1:A:1112:PRO:HD2	2.56	0.41
1:B:1616:MET:HE2	1:B:1616:MET:HB3	1.83	0.41
1:A:810:TYR:HB2	1:A:904:PHE:CZ	2.55	0.41
1:A:1561:GLU:HB2	1:A:1616:MET:SD	2.60	0.41
1:A:1724:ALA:N	1:A:1746:ARG:HH22	2.18	0.41
1:A:199:LYS:O	1:A:510:ARG:NH1	2.53	0.41
1:B:937:LYS:HB2	1:B:1053:LEU:HD21	2.02	0.41
1:B:1753:PHE:HB3	1:B:1782:LEU:HD21	2.02	0.41
1:A:59:LYS:HD3	1:A:59:LYS:N	2.35	0.41
1:A:985:THR:C	1:A:986:PHE:HD1	2.28	0.41
1:A:1001:ARG:NH1	6:A:2012:HOH:O	2.53	0.41
1:B:388:LEU:HB2	1:B:438:SER:OG	2.20	0.41
1:B:616:LEU:HD11	1:B:678:LEU:HD12	2.02	0.41
1:A:730:ILE:HD13	1:A:730:ILE:HA	1.90	0.41
1:B:819:ASP:HB3	1:B:822:GLN:HB2	2.03	0.41
1:B:1325:GLN:O	1:B:1329:VAL:HG23	2.21	0.41
1:A:499:TYR:HB2	1:A:502:ILE:HG12	2.02	0.41
1:A:651:PRO:O	1:A:655:ILE:HG13	2.21	0.41
1:A:700:GLU:HG3	1:A:761:LYS:HD3	2.03	0.41
1:A:1406:LEU:HB2	1:A:1453:ILE:HD13	2.03	0.41
1:A:1526:LYS:H	1:A:1526:LYS:HG3	1.66	0.41
1:A:1578:ALA:O	1:A:1582:GLU:HG3	2.21	0.41
1:B:64:ARG:HE	1:B:64:ARG:HB3	1.64	0.41
1:B:958:GLN:CD	1:B:1090:ASN:HA	2.46	0.41
1:B:1284:MET:HE2	1:B:1284:MET:HB3	1.85	0.41
1:B:1401:GLN:C	1:B:1403:ASP:H	2.28	0.41
1:A:74:PRO:HA	1:A:98:VAL:HG12	2.03	0.41
1:A:294:TYR:OH	1:A:358:ALA:O	2.23	0.41
1:A:707:TRP:HB3	1:A:716:MET:HE3	2.02	0.41
1:A:1255:ARG:NH1	1:A:1258:GLN:OE1	2.54	0.41
1:A:1617:ASP:N	1:A:1617:ASP:OD1	2.53	0.41
1:A:1622:ILE:H	1:A:1627:ILE:HD11	1.86	0.41
1:A:1680:ARG:H	1:A:1680:ARG:HG2	1.67	0.41
1:B:291:ARG:HG2	1:B:295:MET:CE	2.45	0.41
1:B:1234:THR:HB	1:B:1237:LYS:HB2	2.02	0.41
1:A:1516:THR:OG1	1:A:1517:ILE:N	2.49	0.40
1:B:450:GLN:HE21	1:B:451:MET:HE2	1.86	0.40
1:B:456:PHE:O	1:B:475:TYR:HB3	2.21	0.40
1:A:1310:ILE:O	1:A:1314:PHE:CD1	2.74	0.40
1:A:796:ILE:HG21	1:A:806:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:PHE:HD2	1:A:1209:LEU:HD23	1.86	0.40
1:A:1532:PRO:HG2	1:A:1611:GLU:CD	2.46	0.40
1:B:1622:ILE:HD13	1:B:1622:ILE:HA	1.94	0.40
1:A:209:PHE:O	1:A:213:VAL:HG23	2.21	0.40
1:A:1629:LEU:HD12	1:A:1629:LEU:H	1.87	0.40
1:B:1741:VAL:O	1:B:1762:LYS:NZ	2.54	0.40
1:A:658:TYR:HE1	1:A:687:LEU:HD23	1.87	0.40

All (2) 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:38:GLN:NE2	1:B:43:GLN:OE1[1_456]	2.12	0.08
1:A:38:GLN:NE2	1:B:43:GLN:NE2[1_456]	2.17	0.03

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	1769/1814 (98%)	1693 (96%)	67 (4%)	9 (0%)	24 54
1	B	1734/1814 (96%)	1640 (95%)	92 (5%)	2 (0%)	48 77
All	All	3503/3628 (97%)	3333 (95%)	159 (4%)	11 (0%)	36 65

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	685	ALA
1	A	1112	PRO
1	A	194	PRO
1	A	198	GLU
1	A	687	LEU

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Mol	Chain	Res	Type
1	B	1653	GLN
1	A	1532	PRO
1	A	688	LEU
1	A	1533	VAL
1	B	845	GLY
1	A	488	ILE

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	1515/1563 (97%)	1485 (98%)	30 (2%)	48 78
1	B	1429/1563 (91%)	1385 (97%)	44 (3%)	35 69
All	All	2944/3126 (94%)	2870 (98%)	74 (2%)	42 74

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	357	LEU
1	A	388	LEU
1	A	418	GLU
1	A	545	ARG
1	A	595	ILE
1	A	618	LYS
1	A	622	ASP
1	A	773	GLU
1	A	789	VAL
1	A	801	VAL
1	A	817	THR
1	A	822	GLN
1	A	908	HIS
1	A	909	ILE
1	A	959	ILE
1	A	1112	PRO

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Mol	Chain	Res	Type
1	A	1168	GLU
1	A	1274	VAL
1	A	1411	TYR
1	A	1622	ILE
1	A	1631	GLU
1	A	1632	ILE
1	A	1641	THR
1	A	1642	ILE
1	A	1647	VAL
1	A	1760	SER
1	A	1761	ILE
1	A	1776	THR
1	A	1787	THR
1	B	12	SER
1	B	32	GLN
1	B	38	GLN
1	B	80	ASN
1	B	96	LYS
1	B	300	SER
1	B	330	SER
1	B	331	GLU
1	B	343	ASP
1	B	388	LEU
1	B	393	PHE
1	B	534	VAL
1	B	545	ARG
1	B	590	ILE
1	B	622	ASP
1	B	686	GLU
1	B	728	ASP
1	B	765	THR
1	B	798	GLN
1	B	811	THR
1	B	840	THR
1	B	908	HIS
1	B	930	GLN
1	B	1032	ASP
1	B	1061	LEU
1	B	1157	ILE
1	B	1189	LEU
1	B	1210	ARG
1	B	1265	GLU

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Mol	Chain	Res	Type
1	B	1274	VAL
1	B	1411	TYR
1	B	1464	ILE
1	B	1489	MET
1	B	1491	ASP
1	B	1494	VAL
1	B	1504	VAL
1	B	1564	ILE
1	B	1595	ILE
1	B	1636	LEU
1	B	1741	VAL
1	B	1747	ILE
1	B	1749	ILE
1	B	1791	ILE
1	B	1797	SER

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

Mol	Chain	Res	Type
1	A	71	ASN
1	A	73	HIS
1	A	80	ASN
1	A	165	HIS
1	A	211	GLN
1	A	227	GLN
1	A	255	GLN
1	A	338	HIS
1	A	432	GLN
1	A	709	HIS
1	A	929	GLN
1	A	1131	ASN
1	A	1134	HIS
1	A	1391	HIS
1	A	1550	HIS
1	A	1618	HIS
1	A	1651	ASN
1	B	26	HIS
1	B	32	GLN
1	B	80	ASN
1	B	240	GLN
1	B	577	ASN
1	B	759	GLN

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Mol	Chain	Res	Type
1	B	767	GLN
1	B	863	GLN
1	B	908	HIS
1	B	929	GLN
1	B	1131	ASN
1	B	1191	GLN
1	B	1550	HIS
1	B	1575	ASN
1	B	1609	ASN
1	B	1736	HIS
1	B	1771	GLN
1	B	1781	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	JQG	B	1902	1	24,29,30	2.39	7 (29%)	30,38,41	1.19	3 (10%)
2	GOL	B	1901	-	5,5,5	0.08	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1902	-	5,5,5	0.08	0	5,5,5	0.33	0
3	JQG	A	1903	1	24,29,30	2.41	7 (29%)	30,38,41	1.37	4 (13%)
2	GOL	A	1901	-	5,5,5	0.10	0	5,5,5	0.29	0
4	A1AMO	A	1904	1	18,24,25	2.57	6 (33%)	21,31,34	1.10	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	JQG	B	1902	1	-	16/38/40/41	-
2	GOL	B	1901	-	-	0/4/4/4	-
2	GOL	A	1902	-	-	0/4/4/4	-
3	JQG	A	1903	1	-	8/38/40/41	-
2	GOL	A	1901	-	-	0/4/4/4	-
4	A1AMO	A	1904	1	-	9/29/31/32	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1902	JQG	C07-N06	5.88	1.47	1.33
3	A	1903	JQG	C07-N06	5.75	1.47	1.33
4	A	1904	A1AMO	C02-N03	5.74	1.47	1.33
4	A	1904	A1AMO	C07-N06	5.68	1.46	1.33
3	A	1903	JQG	C11-N10	5.66	1.46	1.33
3	A	1903	JQG	C02-N03	5.60	1.46	1.33
4	A	1904	A1AMO	C11-N10	5.52	1.46	1.33
3	B	1902	JQG	C02-N03	5.51	1.46	1.33
3	B	1902	JQG	C11-N10	5.40	1.46	1.33
3	B	1902	JQG	C30-N29	4.18	1.47	1.33
3	A	1903	JQG	C30-N29	4.11	1.46	1.33
3	B	1902	JQG	O23-C11	-2.50	1.18	1.23
4	A	1904	A1AMO	O23-C11	-2.45	1.18	1.23
3	A	1903	JQG	O01-C02	-2.44	1.18	1.23
3	B	1902	JQG	O01-C02	-2.44	1.18	1.23
3	A	1903	JQG	O23-C11	-2.37	1.18	1.23
4	A	1904	A1AMO	O01-C02	-2.31	1.18	1.23
3	A	1903	JQG	O24-C07	-2.09	1.19	1.23
4	A	1904	A1AMO	O24-C07	-2.03	1.19	1.23
3	B	1902	JQG	O24-C07	-2.01	1.19	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1903	JQG	C25-C02-N03	3.90	122.81	116.38
3	B	1902	JQG	C25-C02-N03	3.20	121.66	116.38
3	A	1903	JQG	C02-C25-N29	2.30	116.58	110.31
3	A	1903	JQG	C04-N03-C02	-2.16	118.66	122.55
3	A	1903	JQG	O01-C02-N03	-2.09	118.57	122.98
3	B	1902	JQG	C08-C09-N10	-2.08	107.57	112.00
3	B	1902	JQG	O01-C02-N03	-2.04	118.67	122.98

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1903	JQG	C12-C14-C16-O17
3	A	1903	JQG	C15-C14-C16-O17
3	A	1903	JQG	C22-C14-C16-O17
3	A	1903	JQG	C02-C25-N29-C30
3	B	1902	JQG	C07-C08-C09-N10
3	B	1902	JQG	C11-C12-C14-C15
3	B	1902	JQG	C11-C12-C14-C16
3	B	1902	JQG	C11-C12-C14-C22
3	B	1902	JQG	O13-C12-C14-C15
3	B	1902	JQG	O13-C12-C14-C16
3	B	1902	JQG	O13-C12-C14-C22
3	B	1902	JQG	C12-C14-C16-O17
3	B	1902	JQG	C15-C14-C16-O17
3	B	1902	JQG	C22-C14-C16-O17
4	A	1904	A1AMO	N03-C02-C25-N29
4	A	1904	A1AMO	O01-C02-C25-N29
4	A	1904	A1AMO	C07-C08-C09-N10
4	A	1904	A1AMO	C12-C14-C16-O17
4	A	1904	A1AMO	C15-C14-C16-O17
4	A	1904	A1AMO	C22-C14-C16-O17
4	A	1904	A1AMO	C08-C07-N06-C05
4	A	1904	A1AMO	O24-C07-N06-C05
3	B	1902	JQG	N29-C25-C26-C28
3	A	1903	JQG	C02-C25-C26-C28
4	A	1904	A1AMO	N03-C04-C05-N06
3	B	1902	JQG	N29-C25-C26-C27
3	A	1903	JQG	C02-C25-C26-C27
3	B	1902	JQG	C26-C25-N29-C30
3	B	1902	JQG	N03-C04-C05-N06

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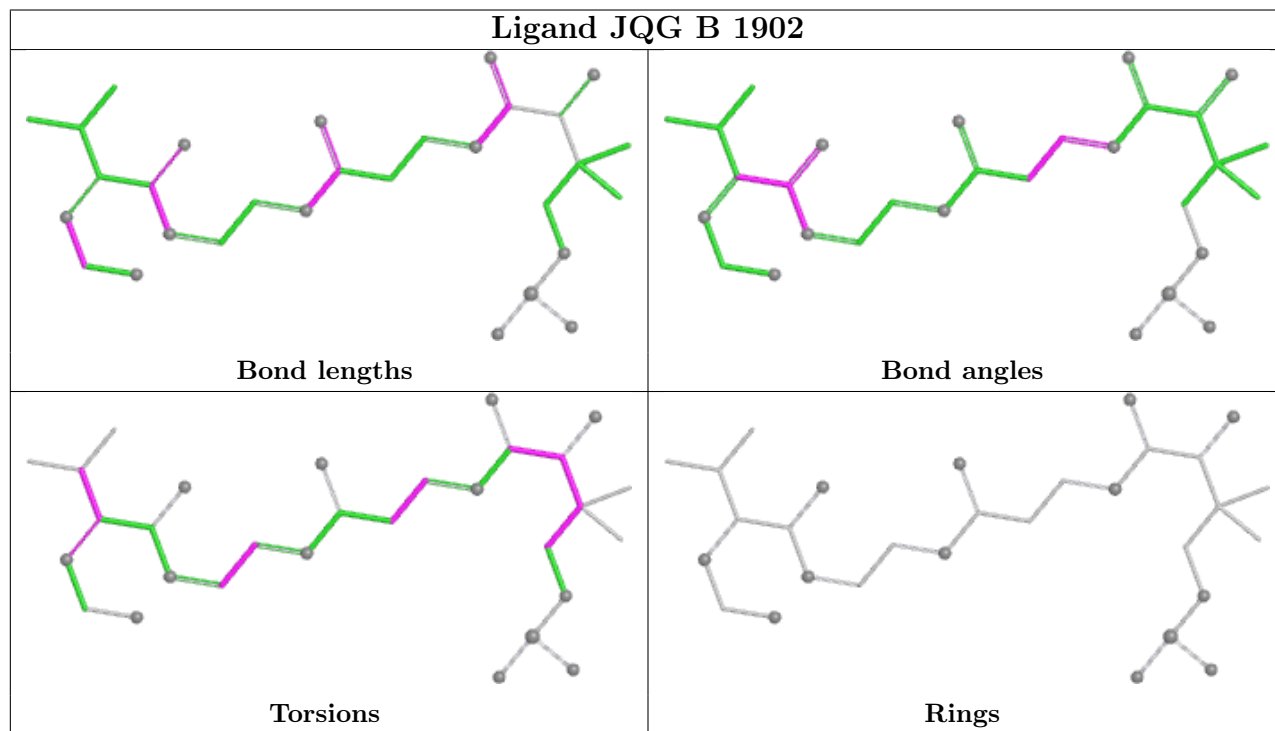
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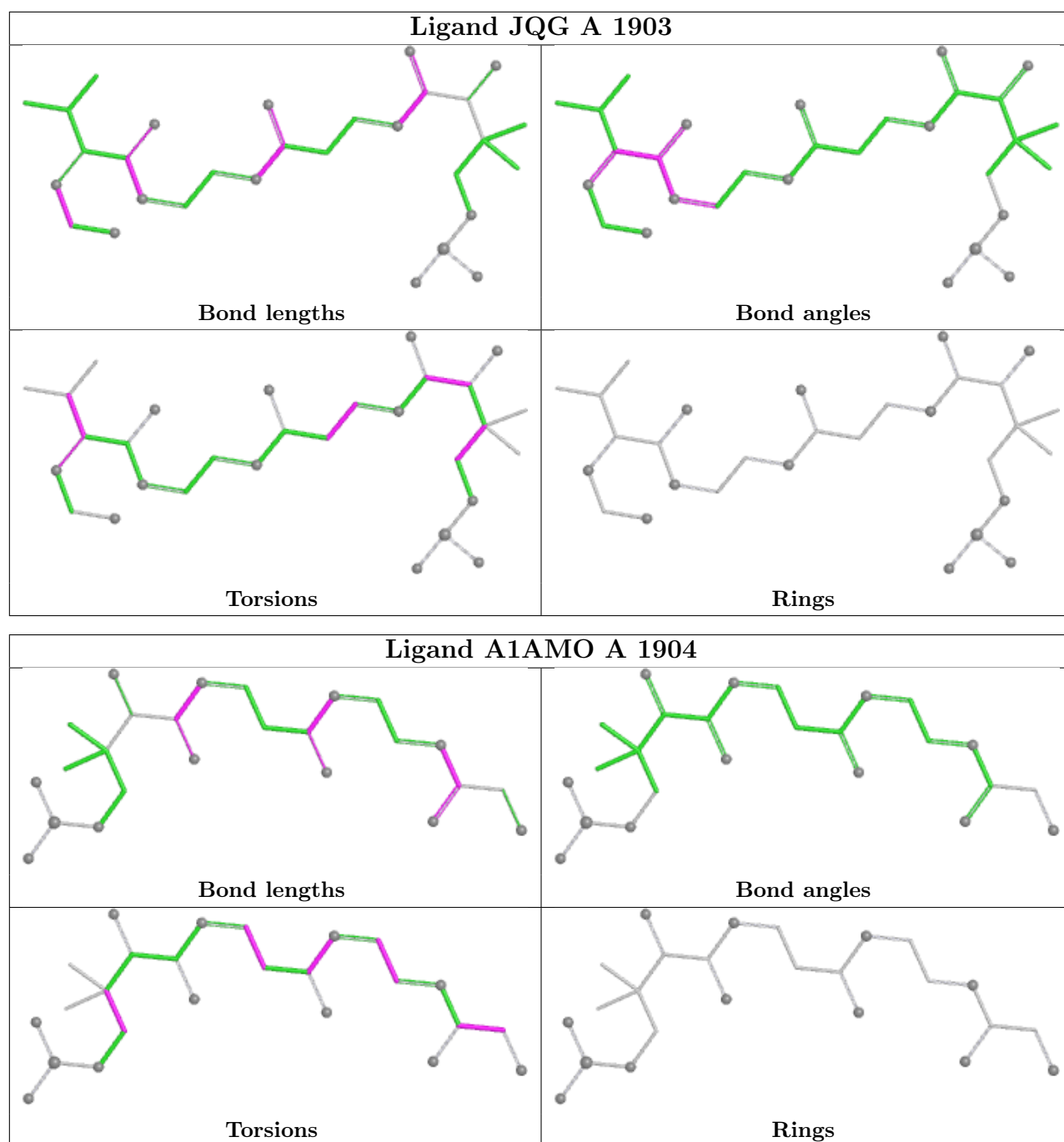
Mol	Chain	Res	Type	Atoms
3	A	1903	JQG	C07-C08-C09-N10
3	B	1902	JQG	C02-C25-C26-C28
3	A	1903	JQG	N10-C11-C12-O13
3	B	1902	JQG	N10-C11-C12-O13

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1774/1814 (97%)	0.34	80 (4%) 38 30	29, 56, 102, 162	1 (0%)
1	B	1746/1814 (96%)	0.42	109 (6%) 26 21	24, 61, 99, 130	0
All	All	3520/3628 (97%)	0.38	189 (5%) 31 24	24, 58, 100, 162	1 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	ALA	7.2
1	A	1724	ALA	6.5
1	A	1646	VAL	5.9
1	B	1726	PRO	5.5
1	B	357	LEU	5.4
1	A	1111[A]	HIS	5.2
1	A	1337	VAL	5.1
1	B	1474	THR	4.9
1	A	685	ALA	4.8
1	A	687	LEU	4.7
1	B	1652	ASP	4.6
1	B	419	ARG	4.4
1	B	1747	ILE	4.4
1	A	357	LEU	4.0
1	B	953	ASP	3.9
1	B	82	GLY	3.9
1	B	1476	ALA	3.9
1	B	1685	TYR	3.8
1	B	1659	LEU	3.5
1	A	1265	GLU	3.5
1	B	74	PRO	3.4
1	B	1473	ARG	3.4
1	B	1630	ASP	3.4
1	B	1678	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1335	ALA	3.4
1	B	1515	ALA	3.4
1	A	1670	THR	3.4
1	B	355	THR	3.4
1	B	1760	SER	3.4
1	B	771	LEU	3.3
1	B	1759	ASP	3.3
1	A	15	ASN	3.3
1	A	1647	VAL	3.2
1	A	622	ASP	3.2
1	A	1645	ALA	3.2
1	A	1689	ALA	3.2
1	A	1725	ALA	3.2
1	B	1677	LEU	3.2
1	A	197	GLY	3.2
1	B	958	GLN	3.2
1	A	1294	ALA	3.1
1	B	1356	LEU	3.1
1	B	1749	ILE	3.1
1	B	1791	ILE	3.1
1	A	355	THR	3.1
1	A	1660	CYS	3.1
1	B	79	TRP	3.0
1	A	1	MET	3.0
1	A	1671	VAL	3.0
1	A	1109	ASN	3.0
1	B	37	ALA	2.9
1	B	1318	GLY	2.9
1	A	1354	PRO	2.9
1	B	1686	MET	2.9
1	A	416	PRO	2.9
1	A	1334	MET	2.9
1	A	1648	VAL	2.9
1	A	1107	GLU	2.8
1	A	1348	ALA	2.8
1	B	1357	VAL	2.8
1	B	1504	VAL	2.8
1	B	959	ILE	2.8
1	A	1652	ASP	2.8
1	B	95	PRO	2.8
1	B	799	GLN	2.8
1	A	1620	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	356	GLY	2.8
1	B	1753	PHE	2.7
1	B	94	THR	2.7
1	B	964	THR	2.7
1	A	1321	LEU	2.7
1	A	1661	ALA	2.7
1	A	198	GLU	2.7
1	A	621	ALA	2.7
1	A	1635	LYS	2.7
1	B	1370	SER	2.7
1	B	1500	VAL	2.7
1	A	623	GLY	2.7
1	A	1274	VAL	2.7
1	B	951	ALA	2.6
1	A	194	PRO	2.6
1	A	772	LEU	2.6
1	B	1050	THR	2.6
1	B	1469	TYR	2.6
1	A	1744	ILE	2.6
1	B	1680	ARG	2.6
1	B	1653	GLN	2.6
1	A	1654	ASN	2.6
1	B	1689	ALA	2.6
1	B	1754	PHE	2.6
1	B	1625	TYR	2.5
1	B	1676	GLU	2.5
1	A	1314	PHE	2.5
1	B	1096	ASP	2.5
1	A	1373	THR	2.5
1	A	1783	PHE	2.5
1	B	1674	LEU	2.5
1	A	1370	SER	2.5
1	A	1655	GLY	2.5
1	B	1527	GLY	2.5
1	A	1234	THR	2.5
1	B	1222	LEU	2.4
1	B	1339	LEU	2.4
1	A	1673	GLN	2.4
1	B	1657	ALA	2.4
1	A	1516	THR	2.4
1	B	1756	LEU	2.4
1	B	1738	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1312	TYR	2.4
1	B	1790	GLN	2.4
1	B	1189	LEU	2.4
1	A	161	GLY	2.4
1	A	1295	GLY	2.4
1	B	1758	GLY	2.4
1	A	419	ARG	2.4
1	B	1453	ILE	2.4
1	B	1744	ILE	2.4
1	B	1672	GLY	2.4
1	A	728	ASP	2.4
1	B	1492	GLU	2.4
1	B	770(A)	ASN	2.3
1	B	1044	GLY	2.3
1	B	1623	ARG	2.3
1	B	697	ASP	2.3
1	B	1314	PHE	2.3
1	B	198	GLU	2.3
1	B	960	ALA	2.3
1	B	849	VAL	2.3
1	B	417	SER	2.3
1	B	1493	LEU	2.3
1	B	1743	GLY	2.3
1	B	1037	ILE	2.3
1	A	1106	ARG	2.3
1	B	307	ASN	2.3
1	B	948	GLU	2.3
1	B	957	GLN	2.3
1	B	1209	LEU	2.3
1	A	1338	VAL	2.3
1	A	1168	GLU	2.2
1	B	1524	LEU	2.2
1	A	196	ARG	2.2
1	B	1238	THR	2.2
1	A	1691	PHE	2.2
1	B	80	ASN	2.2
1	B	1106	ARG	2.2
1	B	487	THR	2.2
1	B	1783	PHE	2.2
1	B	1505	LYS	2.2
1	B	1098	ILE	2.2
1	B	1750	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	680	ASP	2.2
1	B	1786	PRO	2.2
1	A	1658	TYR	2.2
1	B	1101	ALA	2.2
1	B	1622	ILE	2.2
1	B	1337	VAL	2.2
1	A	1267	GLY	2.2
1	A	1400	LEU	2.2
1	A	37	ALA	2.2
1	A	1332	ALA	2.2
1	B	728	ASP	2.1
1	A	1320	LYS	2.1
1	B	161	GLY	2.1
1	B	1681	GLU	2.1
1	B	1313	ILE	2.1
1	A	1261	HIS	2.1
1	A	1322	VAL	2.1
1	A	1105	LYS	2.1
1	B	1190	ASP	2.1
1	B	962	TRP	2.1
1	A	1343	SER	2.1
1	A	1477	ASN	2.1
1	B	1338	VAL	2.1
1	B	971	PRO	2.1
1	B	1784	LEU	2.1
1	B	1319	ALA	2.1
1	A	686	GLU	2.1
1	B	1312	TYR	2.1
1	A	1303	PRO	2.1
1	B	1084	LEU	2.1
1	B	1617	ASP	2.1
1	A	945	TRP	2.1
1	A	352	SER	2.0
1	A	1371	GLY	2.0
1	B	1310	ILE	2.0
1	A	1336	GLU	2.0
1	A	1104	VAL	2.0
1	B	1322	VAL	2.0
1	A	968	GLY	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](#)

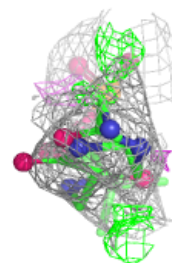
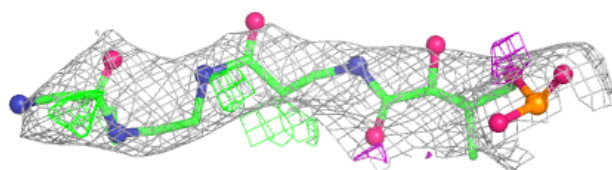
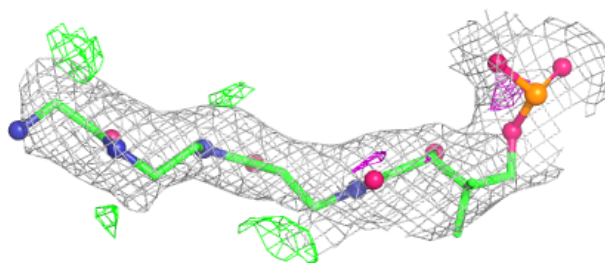
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MN	B	1905	1/1	0.63	0.41	224,224,224,224	0
5	MN	A	1905	1/1	0.78	0.15	107,107,107,107	0
2	GOL	A	1902	6/6	0.81	0.18	36,52,77,84	0
2	GOL	B	1901	6/6	0.84	0.12	34,39,55,76	0
5	MN	B	1904	1/1	0.88	0.12	140,140,140,140	0
4	A1AMO	A	1904	25/26	0.88	0.18	71,83,104,111	0
5	MN	B	1903	1/1	0.93	0.08	79,79,79,79	0
2	GOL	A	1901	6/6	0.93	0.13	38,49,59,62	0
3	JQG	B	1902	30/31	0.93	0.14	42,61,77,86	0
3	JQG	A	1903	30/31	0.97	0.10	30,43,73,77	0

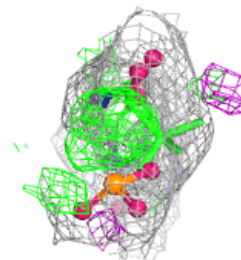
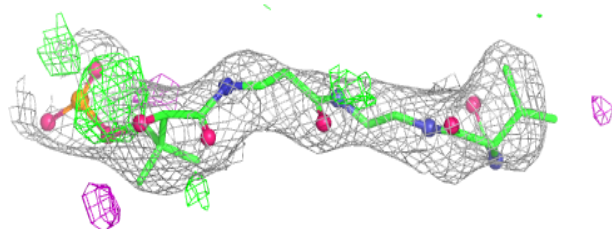
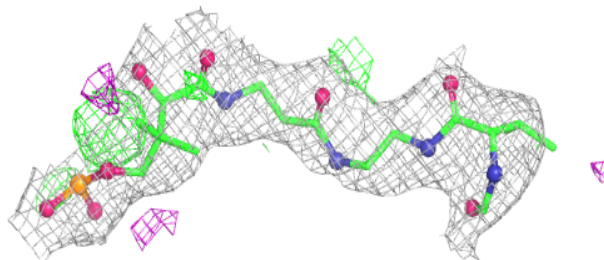
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

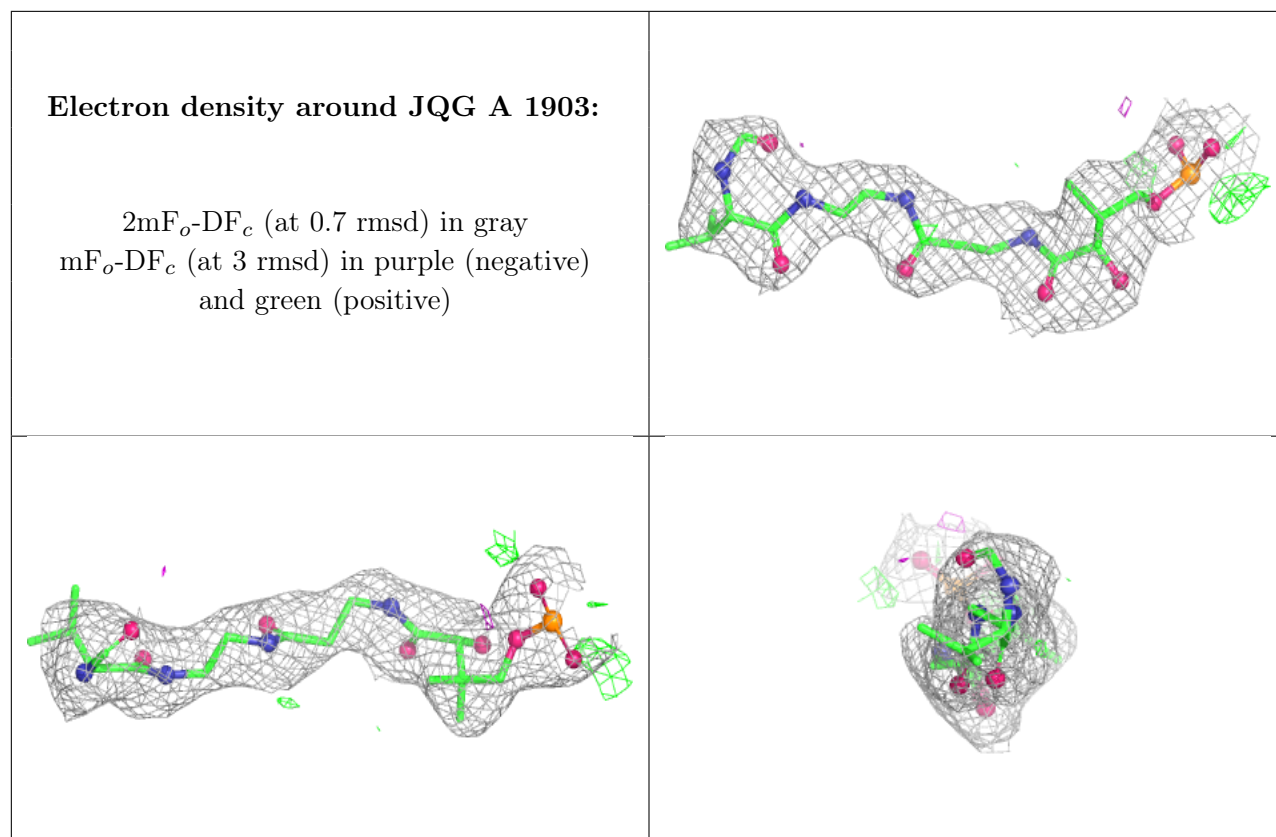
Electron density around A1AMO A 1904:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around JQG B 1902:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.