Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2024 – 10:40 AM EST

PDB ID	:	9BE3
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

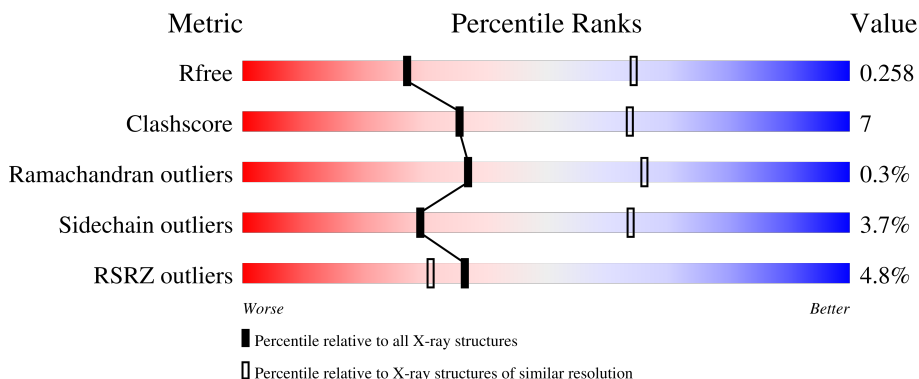|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
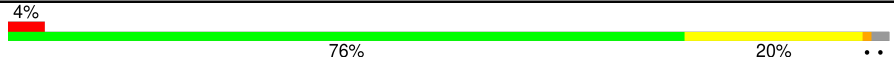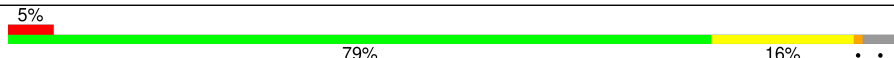*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.258
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		3.7%
RSRZ outliers		4.8%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 <=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%￼￼20%￼・・
1	B	1814	5%￼￼79%￼￼16%￼・・

2 Entry composition ⓘ

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
1	A	1774	Total 14120	C 9015	N 2413	O 2634	S 58	0	1	0
1	B	1746	Total 13627	C 8719	N 2307	O 2544	S 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).
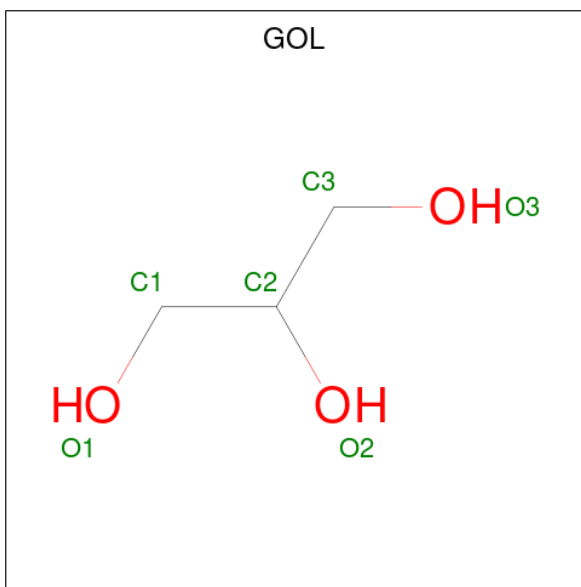
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

- 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)-l^{6}-phosphanyl]oxy-butanamide (three-letter code: JQG) (formula: $C_{17}H_{32}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).
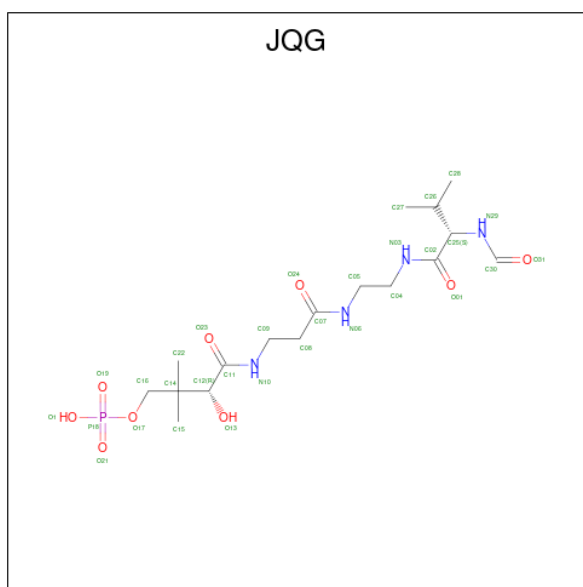
JQG

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

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

A1AMO
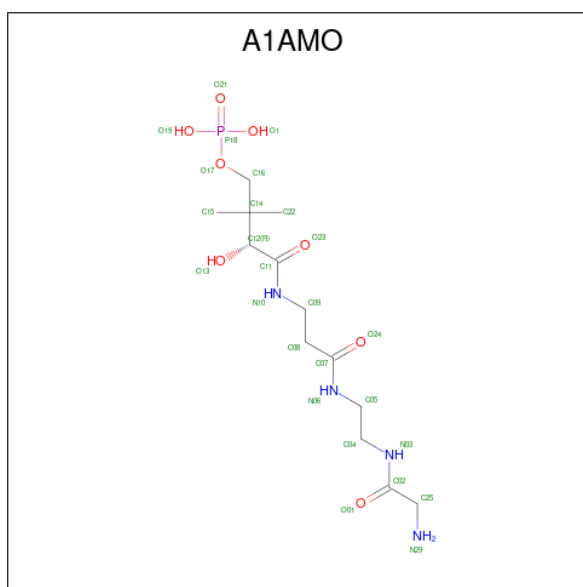
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	13	4	7	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	277	Total O 277 277	0	0
6	B	224	Total O 224 224	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
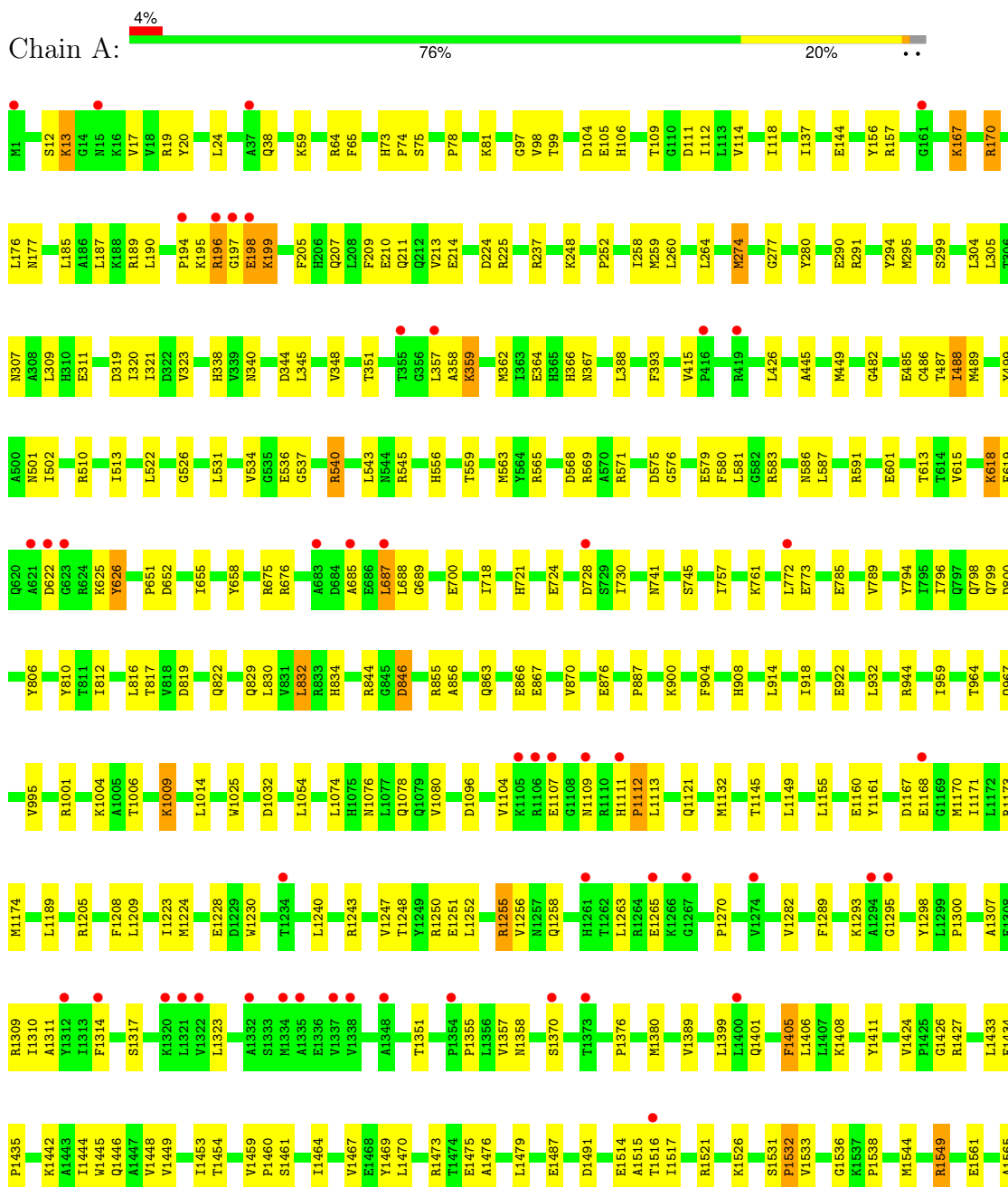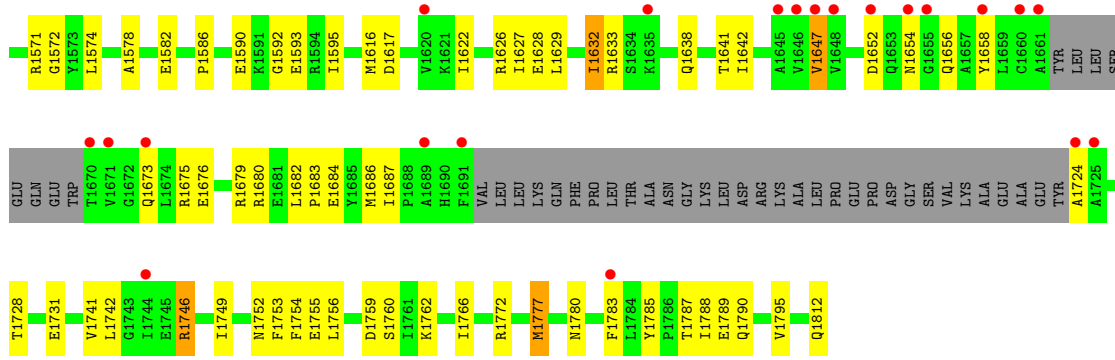
• Molecule 1: Linear gramicidin synthase subunit A
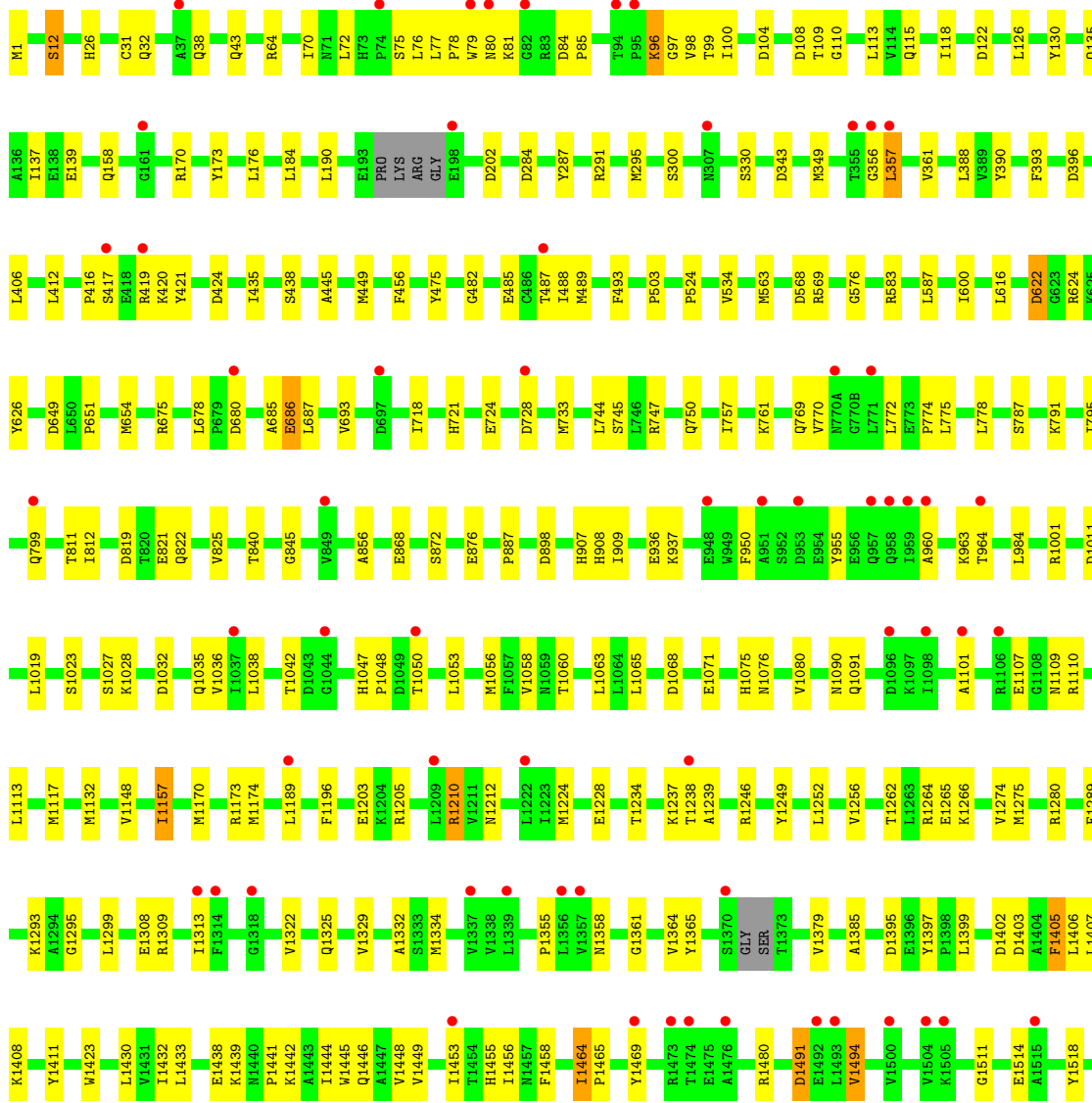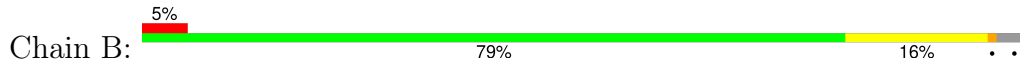
4 Data and refinement statistics (i)

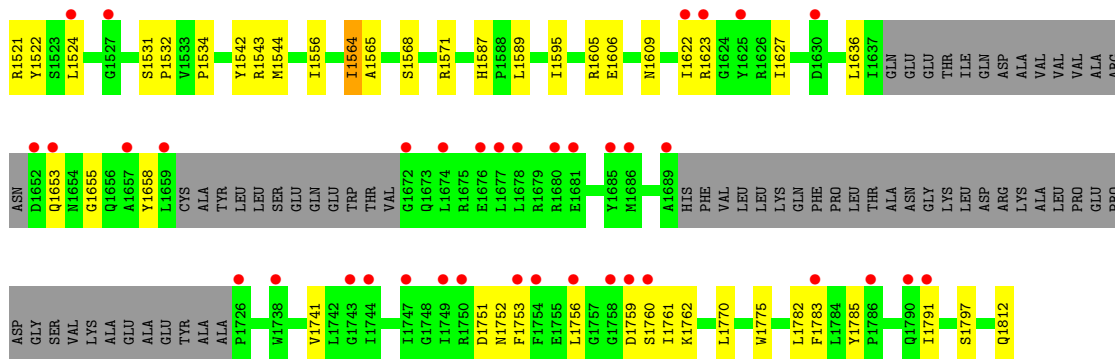| Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	184.82Å 427.90Å 77.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.90 48.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.74-2.90) 98.9 (48.74-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.91Å)	Xtriage
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	134115 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.26	0/14430	0.50	0/19594
1	B	0.26	0/13926	0.49	3/18947 (0.0%)
All	All	0.26	0/28356	0.49	3/38541 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1334	MET	CG-SD-CE	5.74	109.39	100.20
1	B	1453	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	B	357	LEU	CA-CB-CG	5.08	126.98	115.30

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 ⓘ

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	233	2
1	B	13627	0	13332	165	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	5	0
6	B	224	0	0	1	0
All	All	28355	0	27381	397	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 7.

All (397) 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:205:PHE:HD2	1:A:274:MET:HE1	1.49	0.77
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:291:ARG:HG2	1:B:295:MET:HE2	1.77	0.65
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1405:PHE:HD1	1:A:1406:LEU:H	1.52	0.57
1:B:173:TYR:HB3	1:B:176:LEU:HD12	1.86	0.57
1:A:259:MET:HE2	1:A:304:LEU:HD21	1.85	0.57
1:A:799:GLN:HG3	1:A:800:ASP:N	2.18	0.56
1:A:205:PHE:CD2	1:A:274:MET:HE1	2.37	0.56
1:B:1076:ASN:O	1:B:1080:VAL:HG23	2.05	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: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:B:202:ASP:N	1:B:202:ASP:OD1	2.39	0.56
1:A:345:LEU:HD11	1:A:362:MET:HE3	1.89	0.55
1:B:721:HIS:HB3	1:B:724:GLU:HB2	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:687:LEU:C	1:A:689:GLY:H	2.12	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:1683:PRO:HD2	1:A:1686:MET:HE2	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:349:MET:HE3	1:B:396:ASP:HA	1.91	0.52
1:B:1531:SER:OG	1:B:1532:PRO:HD3	2.10	0.52
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:1626:ARG:HH22	1:A:1628:GLU:CD	2.13	0.51
1:A:1676:GLU:HA	1:A:1679:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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	1.78	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: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:B:1060:THR:HG22	1:B:1117:MET:HE1	1.96	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
1:A:1759:ASP:H	1:A:1762:LYS:HG3	1.80	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:B:1028:LYS:NZ	1:B:1196:PHE:O	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:274:MET:HE3	1:A:274:MET:HB3	1.83	0.46
1:A:575:ASP:N	1:A:575:ASP:OD1	2.48	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: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:A:1654:ASN:C	1:A:1656:GLN:H	2.19	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: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:1096:ASP:OD1	1:A:1096:ASP:N	2.48	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:B:291:ARG:HG2	1:B:295:MET:CE	2.45	0.45
1:A:1173:ARG:NH1	6:A:2009:HOH:O	2.50	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1516:THR:OG1	1:A:1517:ILE:N	2.49	0.44
1:B:1113:LEU:HD23	1:B:1113:LEU:HA	1.77	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:362:MET:HE2	1:A:540:ARG:HB3	1.99	0.44
1:A:618:LYS:HZ1	1:A:676:ARG:HH22	1.66	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: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: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: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:A:1380:MET:HE3	1:A:1571:ARG:HD2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1770:LEU:HB3	1:B:1775:TRP:HB2	2.01	0.43
1:A:1256:VAL:HG11	1:A:1289:PHE:HB3	2.00	0.42
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:1075:HIS:C	1:B:1075:HIS:CD2	2.93	0.42
1:A:1459:VAL:HG22	1:A:1460:PRO:O	2.19	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:291:ARG:NH1	1:A:295:MET:HE2	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:CYS:HA	1:A:537:GLY:O	2.19	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: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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1234:THR:HB	1:B:1237:LYS:HB2	2.02	0.41
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
1:A:1208:PHE:HD2	1:A:1209:LEU:HD23	1.86	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:356:GLY:C	1:B:357:LEU:HD23	2.41	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
1:A:1515:ALA:C	1:A:1516:THR:HG1	2.20	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 ⓘ

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	1769/1814 (98%)	1693 (96%)	67 (4%)	9 (0%)	25	56
1	B	1734/1814 (96%)	1640 (95%)	92 (5%)	2 (0%)	48	77
All	All	3503/3628 (97%)	3333 (95%)	159 (4%)	11 (0%)	37	66

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
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 ⓘ

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%)	1459 (96%)	56 (4%)	29	64
1	B	1429/1563 (91%)	1375 (96%)	54 (4%)	28	63
All	All	2944/3126 (94%)	2834 (96%)	110 (4%)	29	64

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	17	VAL
1	A	167	LYS
1	A	170	ARG
1	A	176	LEU
1	A	196	ARG
1	A	199	LYS
1	A	237	ARG
1	A	274	MET
1	A	290	GLU
1	A	357	LEU
1	A	359	LYS
1	A	393	PHE

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Mol	Chain	Res	Type
1	A	540	ARG
1	A	545	ARG
1	A	565	ARG
1	A	618	LYS
1	A	622	ASP
1	A	626	TYR
1	A	675	ARG
1	A	728	ASP
1	A	745	SER
1	A	773	GLU
1	A	789	VAL
1	A	817	THR
1	A	832	LEU
1	A	844	ARG
1	A	846	ASP
1	A	855	ARG
1	A	908	HIS
1	A	959	ILE
1	A	1009	LYS
1	A	1168	GLU
1	A	1205	ARG
1	A	1224	MET
1	A	1243	ARG
1	A	1250	ARG
1	A	1255	ARG
1	A	1265	GLU
1	A	1309	ARG
1	A	1405	PHE
1	A	1411	TYR
1	A	1491	ASP
1	A	1549	ARG
1	A	1632	ILE
1	A	1638	GLN
1	A	1641	THR
1	A	1642	ILE
1	A	1647	VAL
1	A	1658	TYR
1	A	1673	GLN
1	A	1760	SER
1	A	1777	MET
1	A	1787	THR
1	A	1789	GLU

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Mol	Chain	Res	Type
1	A	1812	GLN
1	B	12	SER
1	B	31	CYS
1	B	32	GLN
1	B	38	GLN
1	B	80	ASN
1	B	96	LYS
1	B	122	ASP
1	B	300	SER
1	B	330	SER
1	B	343	ASP
1	B	393	PHE
1	B	424	ASP
1	B	534	VAL
1	B	563	MET
1	B	622	ASP
1	B	649	ASP
1	B	680	ASP
1	B	686	GLU
1	B	728	ASP
1	B	733	MET
1	B	761	LYS
1	B	778	LEU
1	B	787	SER
1	B	811	THR
1	B	840	THR
1	B	908	HIS
1	B	1011	ASP
1	B	1027	SER
1	B	1032	ASP
1	B	1035	GLN
1	B	1056	MET
1	B	1090	ASN
1	B	1091	GLN
1	B	1157	ILE
1	B	1189	LEU
1	B	1205	ARG
1	B	1210	ARG
1	B	1274	VAL
1	B	1308	GLU
1	B	1395	ASP
1	B	1397	TYR

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Mol	Chain	Res	Type
1	B	1402	ASP
1	B	1405	PHE
1	B	1411	TYR
1	B	1458	PHE
1	B	1464	ILE
1	B	1491	ASP
1	B	1494	VAL
1	B	1521	ARG
1	B	1564	ILE
1	B	1636	LEU
1	B	1785	TYR
1	B	1791	ILE
1	B	1797	SER

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

Mol	Chain	Res	Type
1	A	165	HIS
1	A	211	GLN
1	A	340	ASN
1	A	432	GLN
1	A	709	HIS
1	A	1618	HIS
1	B	80	ASN
1	B	929	GLN
1	B	1035	GLN
1	B	1575	ASN
1	B	1609	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 ⓘ

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	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%)
4	A1AMO	A	1904	1	18,24,25	2.57	6 (33%)	21,31,34	1.10	0
2	GOL	A	1901	-	5,5,5	0.10	0	5,5,5	0.29	0
2	GOL	B	1901	-	5,5,5	0.08	0	5,5,5	0.39	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	A	1902	-	-	0/4/4/4	-
3	JQG	A	1903	1	-	8/38/40/41	-
4	A1AMO	A	1904	1	-	9/29/31/32	-
2	GOL	A	1901	-	-	0/4/4/4	-
2	GOL	B	1901	-	-	0/4/4/4	-

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms
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
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 then 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.

Ligand JQG B 1902

Bond lengths

Bond angles

Torsions

Rings

Ligand JQG A 1903

Bond lengths

Bond angles

Torsions

Rings

Ligand A1AMO A 1904
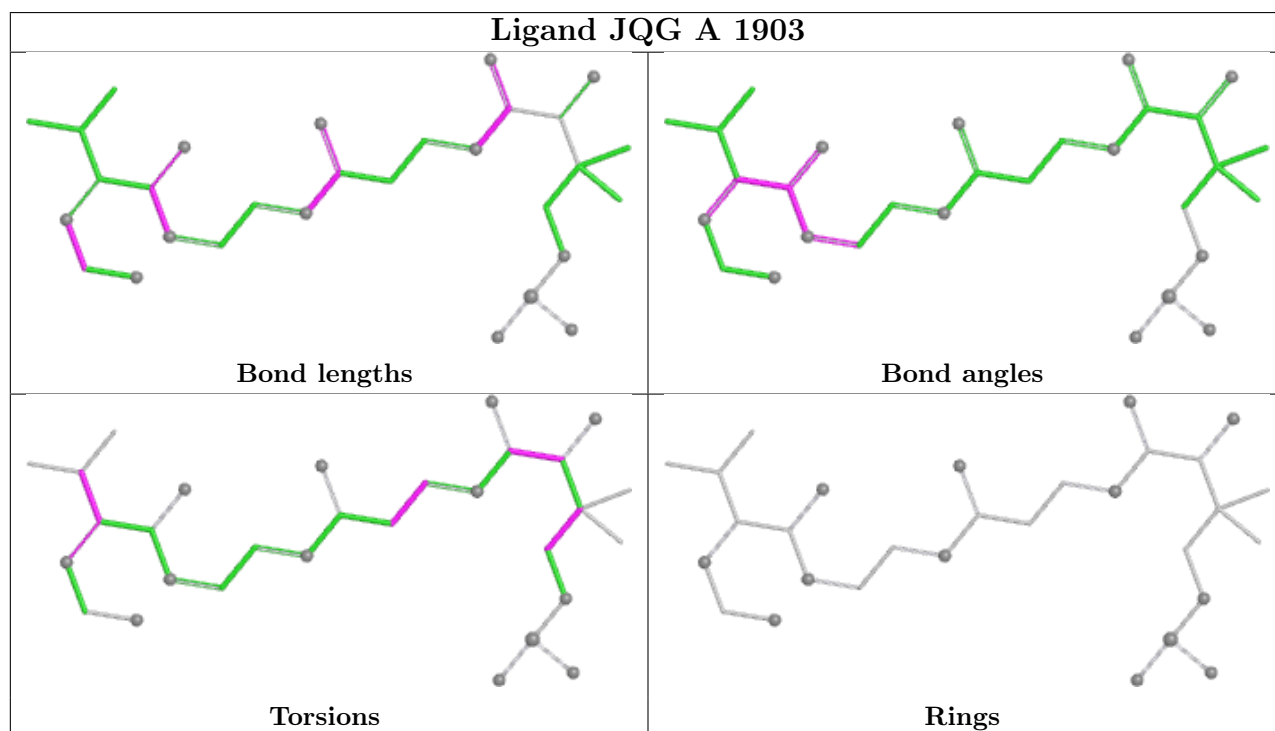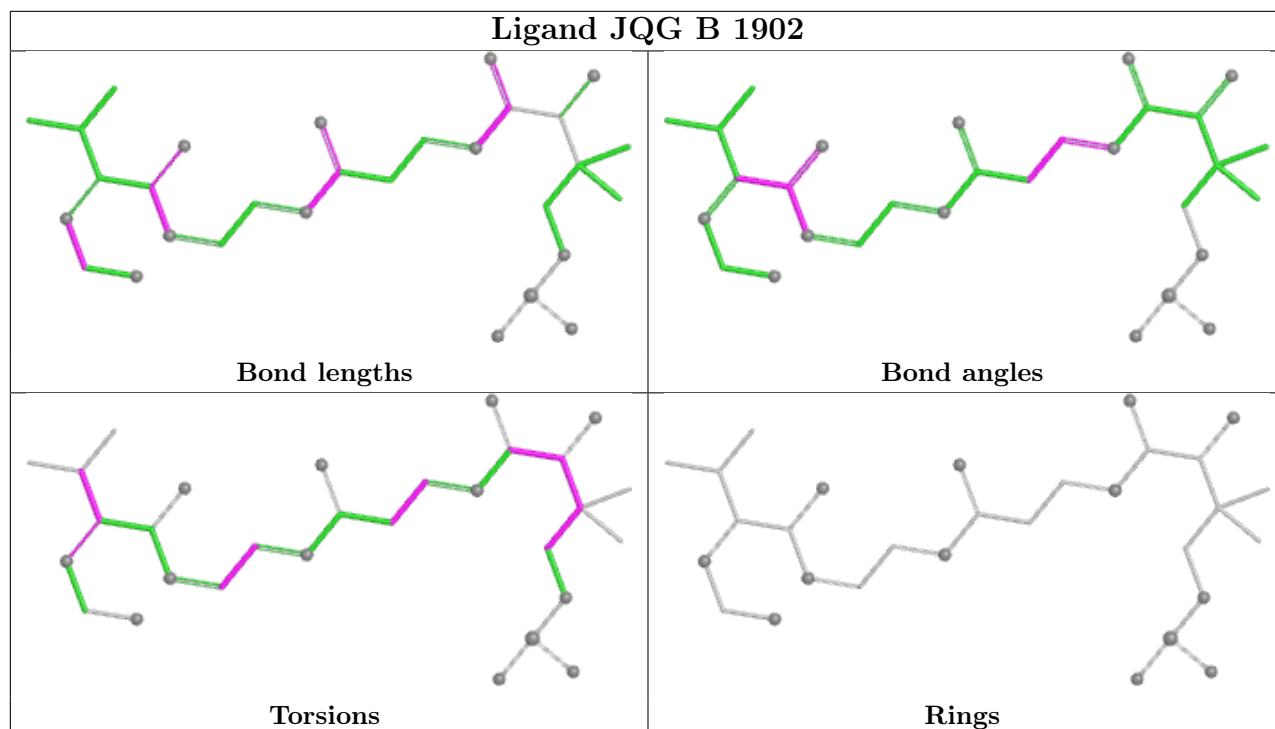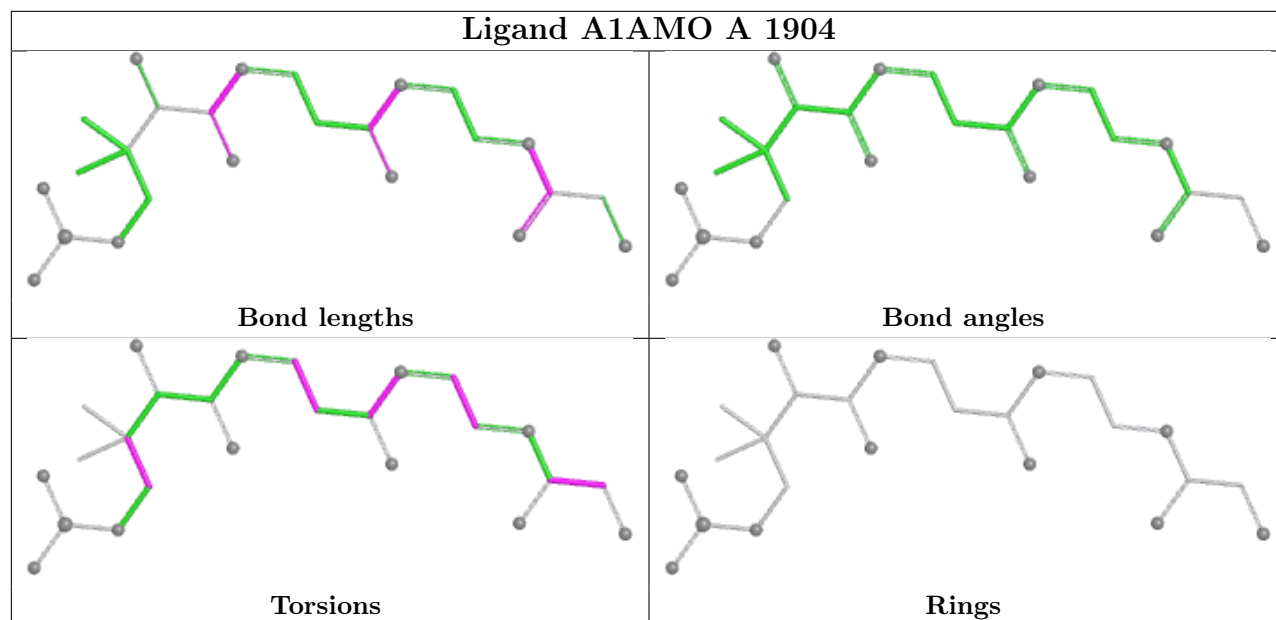
5.7 Other polymers ⓘ

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	1774/1814 (97%)	0.20	70 (3%)	44	37	29, 56, 102, 162	1 (0%)
1	B	1746/1814 (96%)	0.27	98 (5%)	31	27	24, 61, 99, 130	0
All	All	3520/3628 (97%)	0.24	168 (4%)	36	31	24, 58, 100, 162	1 (0%)

All (168) 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	5.4
1	B	357	LEU	5.3
1	A	1111[A]	HIS	5.1
1	A	1337	VAL	5.0
1	B	1474	THR	4.8
1	A	685	ALA	4.7
1	B	1652	ASP	4.6
1	A	687	LEU	4.6
1	B	419	ARG	4.4
1	B	1747	ILE	4.3
1	A	357	LEU	3.9
1	B	953	ASP	3.8
1	B	82	GLY	3.8
1	B	1476	ALA	3.8
1	B	1685	TYR	3.6
1	A	1265	GLU	3.5
1	B	1659	LEU	3.4
1	B	1473	ARG	3.4
1	B	74	PRO	3.3
1	B	1630	ASP	3.3
1	A	1335	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1515	ALA	3.3
1	A	1670	THR	3.3
1	B	355	THR	3.3
1	B	1678	LEU	3.3
1	B	1760	SER	3.3
1	A	15	ASN	3.2
1	B	1759	ASP	3.2
1	B	771	LEU	3.2
1	A	1647	VAL	3.1
1	A	622	ASP	3.1
1	A	1645	ALA	3.1
1	A	1689	ALA	3.1
1	A	1725	ALA	3.1
1	B	958	GLN	3.1
1	B	1677	LEU	3.1
1	A	197	GLY	3.1
1	A	1294	ALA	3.1
1	A	355	THR	3.0
1	B	1749	ILE	3.0
1	B	1791	ILE	3.0
1	B	1356	LEU	3.0
1	A	1660	CYS	2.9
1	A	1109	ASN	2.9
1	A	1671	VAL	2.9
1	A	1	MET	2.9
1	B	79	TRP	2.9
1	B	37	ALA	2.8
1	B	1318	GLY	2.8
1	A	1354	PRO	2.8
1	B	1686	MET	2.8
1	A	1107	GLU	2.8
1	A	1648	VAL	2.8
1	A	416	PRO	2.7
1	A	1334	MET	2.7
1	A	1348	ALA	2.7
1	B	1357	VAL	2.7
1	B	1504	VAL	2.7
1	B	959	ILE	2.7
1	B	799	GLN	2.7
1	A	1652	ASP	2.7
1	A	1620	VAL	2.7
1	B	95	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	356	GLY	2.7
1	A	198	GLU	2.6
1	B	94	THR	2.6
1	B	964	THR	2.6
1	A	1635	LYS	2.6
1	A	1661	ALA	2.6
1	A	621	ALA	2.6
1	A	1321	LEU	2.6
1	B	1753	PHE	2.6
1	B	1370	SER	2.6
1	B	1500	VAL	2.6
1	A	1274	VAL	2.6
1	B	951	ALA	2.5
1	A	623	GLY	2.5
1	A	194	PRO	2.5
1	B	1680	ARG	2.5
1	A	772	LEU	2.5
1	B	1050	THR	2.5
1	A	1744	ILE	2.5
1	B	1653	GLN	2.5
1	B	1676	GLU	2.5
1	A	1654	ASN	2.5
1	B	1689	ALA	2.5
1	B	1469	TYR	2.5
1	B	1096	ASP	2.4
1	B	1754	PHE	2.4
1	A	1373	THR	2.4
1	B	1625	TYR	2.4
1	A	1314	PHE	2.4
1	A	1370	SER	2.4
1	A	1783	PHE	2.4
1	A	1234	THR	2.4
1	A	1673	GLN	2.3
1	B	1674	LEU	2.3
1	A	1655	GLY	2.3
1	B	1527	GLY	2.3
1	B	1657	ALA	2.3
1	A	419	ARG	2.3
1	A	1516	THR	2.3
1	B	1222	LEU	2.3
1	B	1339	LEU	2.3
1	B	1790	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1756	LEU	2.3
1	B	1492	GLU	2.3
1	B	1623	ARG	2.3
1	B	1189	LEU	2.3
1	A	1312	TYR	2.3
1	A	161	GLY	2.3
1	A	1295	GLY	2.3
1	B	1758	GLY	2.3
1	B	1453	ILE	2.3
1	B	1744	ILE	2.3
1	B	198	GLU	2.3
1	B	1738	TRP	2.3
1	A	728	ASP	2.3
1	B	770(A)	ASN	2.2
1	B	1672	GLY	2.2
1	B	960	ALA	2.2
1	B	697	ASP	2.2
1	B	849	VAL	2.2
1	B	1044	GLY	2.2
1	A	1106	ARG	2.2
1	B	417	SER	2.2
1	B	1314	PHE	2.2
1	B	948	GLU	2.2
1	B	1493	LEU	2.2
1	B	1037	ILE	2.2
1	B	1743	GLY	2.2
1	B	957	GLN	2.2
1	A	196	ARG	2.2
1	B	307	ASN	2.2
1	A	1168	GLU	2.2
1	A	1338	VAL	2.2
1	B	1106	ARG	2.1
1	B	1209	LEU	2.1
1	B	1238	THR	2.1
1	B	1750	ARG	2.1
1	B	1505	LYS	2.1
1	B	1524	LEU	2.1
1	B	80	ASN	2.1
1	B	487	THR	2.1
1	B	1098	ILE	2.1
1	A	1691	PHE	2.1
1	B	680	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1101	ALA	2.1
1	B	1786	PRO	2.1
1	B	1622	ILE	2.1
1	B	1337	VAL	2.1
1	A	1320	LYS	2.1
1	B	1783	PHE	2.1
1	A	37	ALA	2.0
1	A	1332	ALA	2.0
1	A	1658	TYR	2.0
1	B	1681	GLU	2.0
1	A	1105	LYS	2.0
1	A	1267	GLY	2.0
1	A	1400	LEU	2.0
1	B	728	ASP	2.0
1	B	1313	ILE	2.0
1	A	1322	VAL	2.0
1	B	161	GLY	2.0
1	A	1261	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
5	MN	B	1905	1/1	0.64	0.40	224,224,224,224	0
5	MN	A	1905	1/1	0.75	0.17	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.
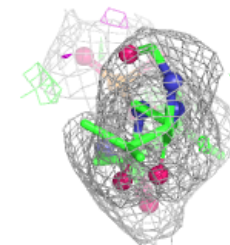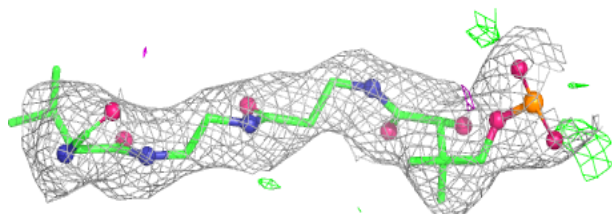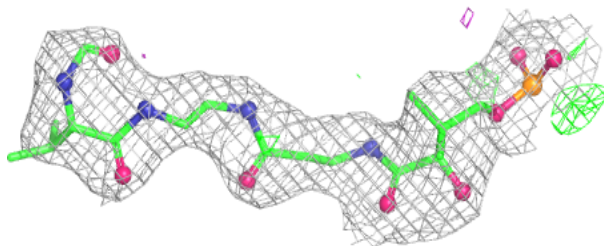
Electron density around A1AMO A 1904:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
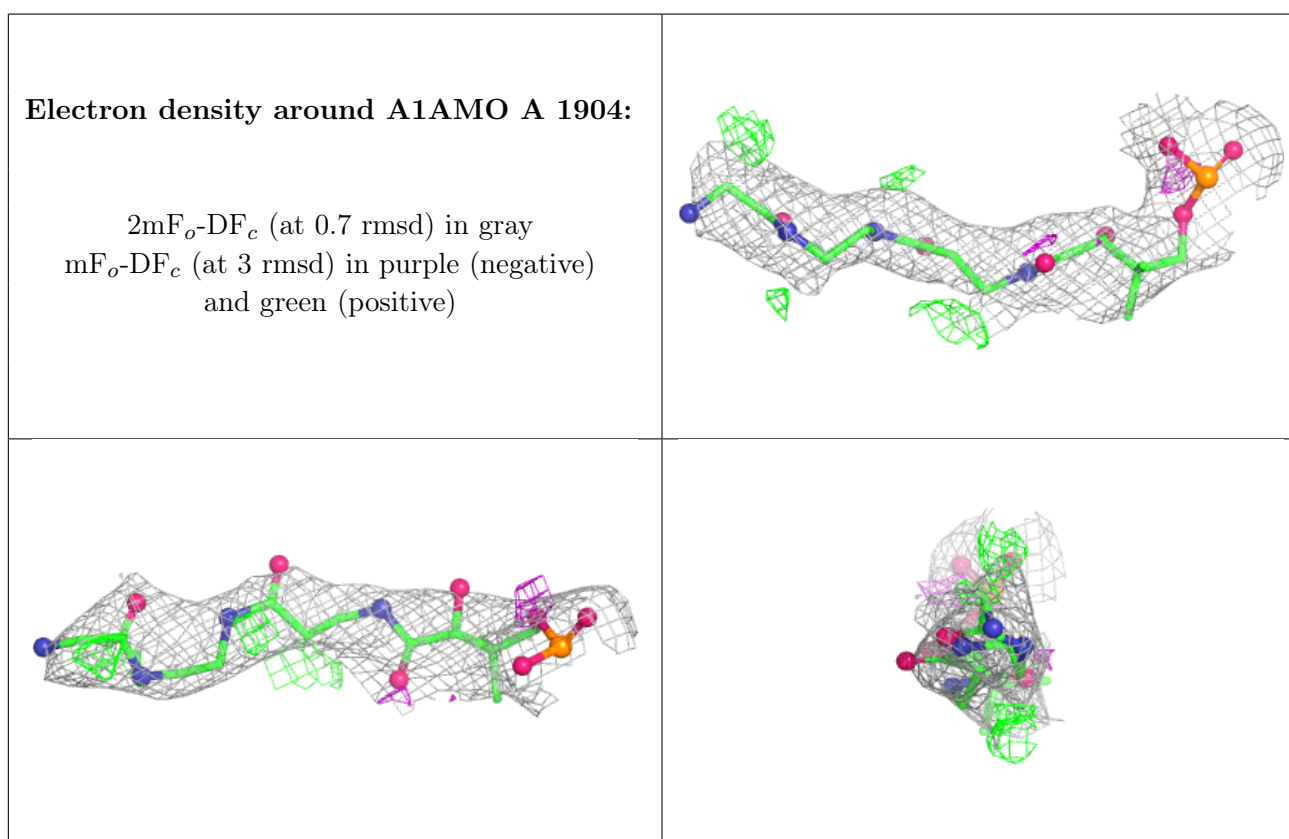
Electron density around JQG B 1902:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
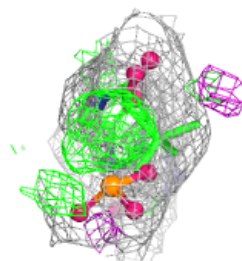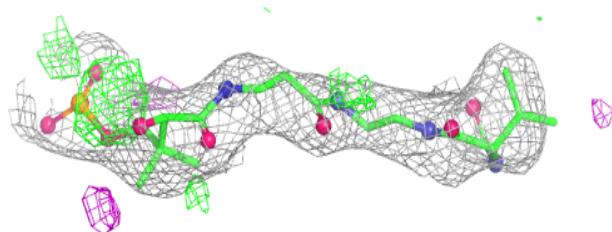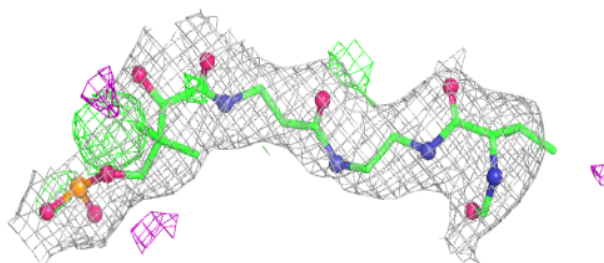
Electron density around JQG A 1903:

$2mF_o$-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 ⓘ

There are no such residues in this entry.