



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:30 PM UTC

PDB ID : 6MFZ / pdb_00006mfz
Title : Crystal structure of dimodular LgrA in a condensation state
Authors : Reimer, J.M.; Eivaskhani, M.; Harb, I.; Schmeing, T.M.
Deposited on : 2018-09-12
Resolution : 6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

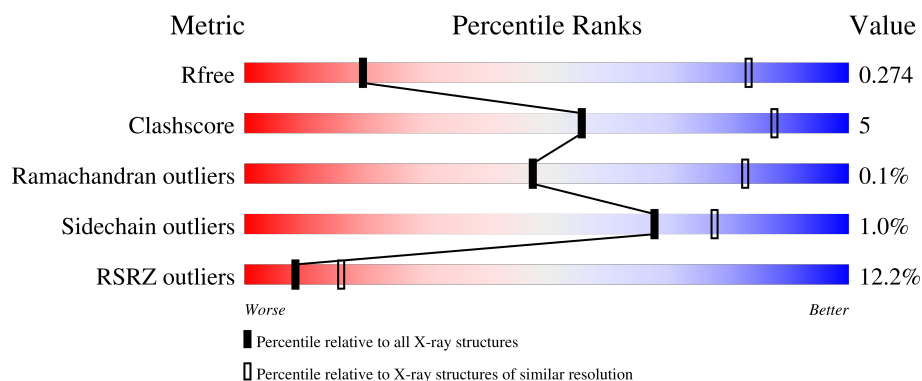
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1814	12% 87% 11%
1	B	1814	4% 29% 68%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18882 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	1789	Total	C	N	O	S	0	0	0
			14226	9089	2430	2649	58			
1	B	585	Total	C	N	O	S	0	0	0
			4648	2958	797	871	22			

There are 26 discrepancies between the modelled and reference sequences:

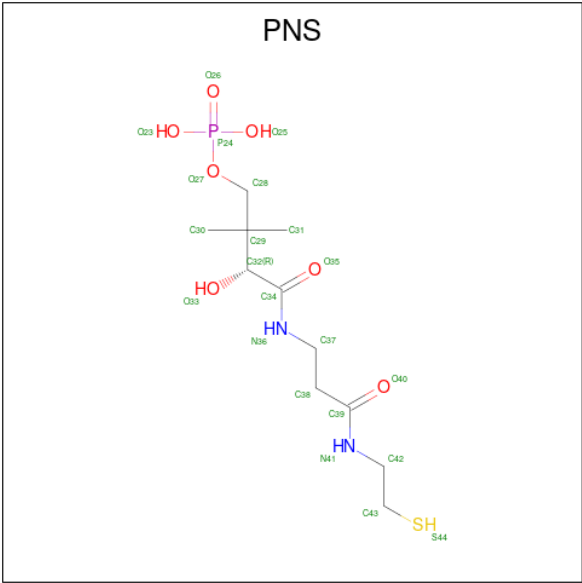
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1804	ALA	-	expression tag	UNP Q70LM7
A	1805	ALA	-	expression tag	UNP Q70LM7
A	1806	ALA	-	expression tag	UNP 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	GLY	-	expression tag	UNP Q70LM7
B	0	ALA	-	expression tag	UNP Q70LM7
B	1	MET	-	expression tag	UNP Q70LM7
B	2	GLY	-	expression tag	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
B	1810	TYR	-	expression tag	UNP Q70LM7
B	1811	PHE	-	expression tag	UNP Q70LM7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1812	GLN	-	expression tag	UNP Q70LM7

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

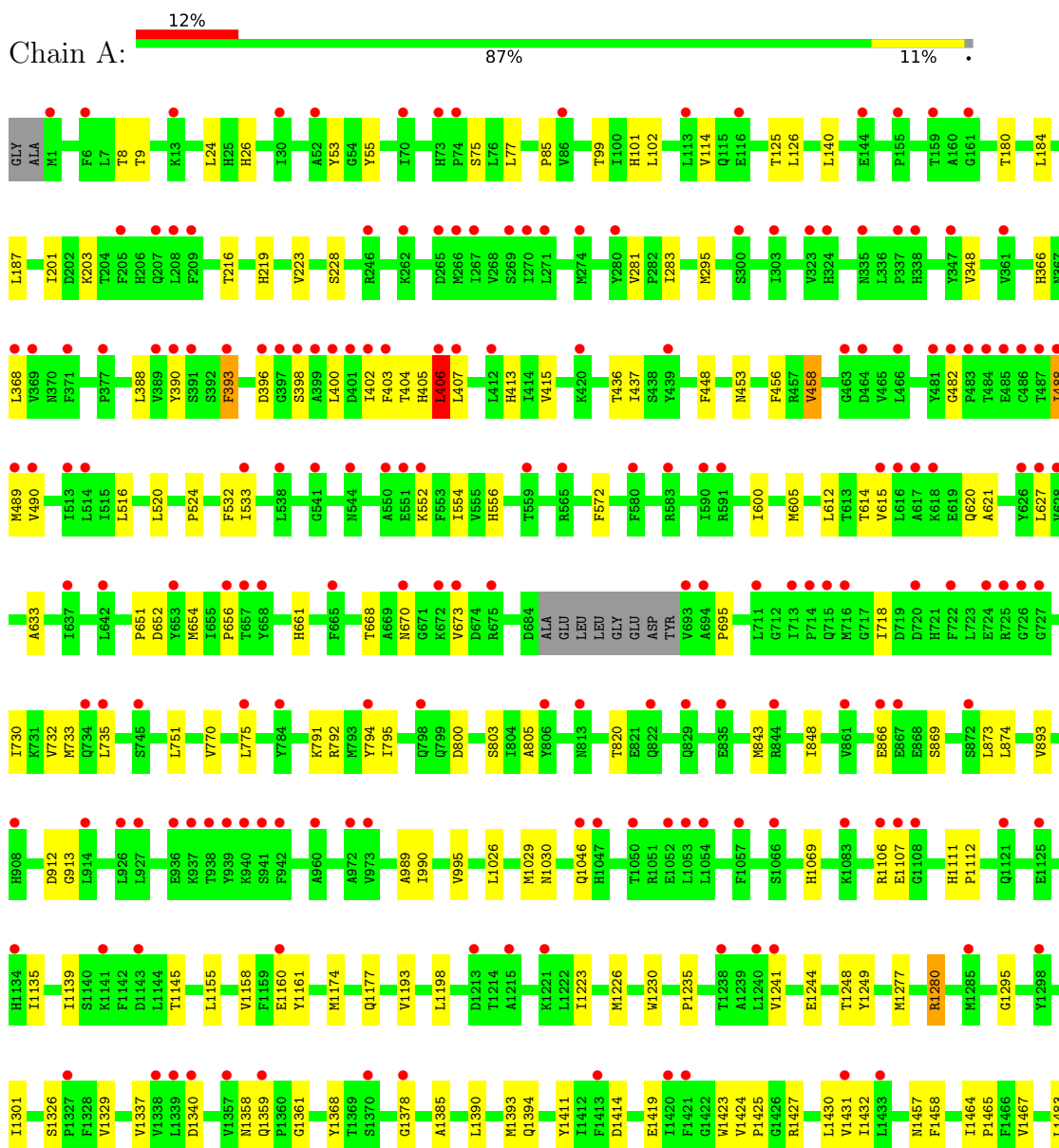


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			4	3	1		
2	A	1	Total	O	P	0	0
			4	3	1		

3 Residue-property plots [i](#)

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

- Molecule 1: Linear gramicidin synthase subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.60Å 262.75Å 249.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.63 – 6.00 78.63 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.63-6.00) 99.8 (78.63-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 6.18Å)	Xtriage
Refinement program	PHENIX (dev_3494: ???)	Depositor
R, R_{free}	0.255 , 0.279 0.254 , 0.274	Depositor DCC
R_{free} test set	894 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	216.9	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 549.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	18882	wwPDB-VP
Average B, all atoms (Å ²)	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PNS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/14537	0.52	15/19739 (0.1%)
1	B	0.21	0/4754	0.39	1/6451 (0.0%)
All	All	0.29	0/19291	0.49	16/26190 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	LEU	CA-C-N	-7.88	110.69	122.83
1	A	406	LEU	C-N-CA	-7.88	110.69	122.83
1	A	1533	VAL	N-CA-C	-7.86	99.77	107.55
1	A	1532	PRO	N-CA-C	-6.96	99.21	110.55
1	A	1518	TYR	N-CA-C	6.79	119.09	110.33
1	A	1745	GLU	N-CA-C	6.25	117.78	110.97
1	A	1046	GLN	N-CA-C	-5.83	104.93	112.68
1	A	1663	LEU	CA-C-N	-5.82	114.50	122.93
1	A	1663	LEU	C-N-CA	-5.82	114.50	122.93
1	A	366	HIS	CA-C-N	5.66	128.13	120.65
1	A	366	HIS	C-N-CA	5.66	128.13	120.65
1	B	226	GLY	N-CA-C	5.56	121.55	114.66
1	A	652	ASP	N-CA-C	5.55	117.33	111.28
1	A	1244	GLU	N-CA-C	5.43	119.90	113.16
1	A	405	HIS	O-C-N	5.11	128.87	122.23
1	A	1623	ARG	N-CA-C	-5.03	100.09	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14226	0	14159	146	0
1	B	4648	0	4573	31	0
2	A	8	0	0	0	0
All	All	18882	0	18732	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (177) 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:1531:SER:HB2	1:A:1532:PRO:HD3	1.35	1.07
1:A:1601:LEU:O	1:A:1613:LEU:HB3	1.55	1.05
1:A:407:LEU:HD23	1:A:407:LEU:O	1.61	1.00
1:A:437:ILE:HG23	1:A:458:VAL:HG12	1.42	0.99
1:A:437:ILE:HG12	1:A:458:VAL:HB	1.44	0.96
1:A:368:LEU:HD21	1:A:403:PHE:CD2	2.07	0.89
1:A:1223:ILE:HG23	1:A:1424:VAL:HG11	1.53	0.88
1:A:1295:GLY:HA2	1:A:1358:ASN:OD1	1.75	0.85
1:A:1752:ASN:HB3	1:A:1755:GLU:HB2	1.58	0.85
1:A:1642:ILE:HD13	1:A:1663:LEU:HD22	1.58	0.84
1:A:24:LEU:O	1:A:26:HIS:HD2	1.61	0.83
1:A:1424:VAL:HB	1:A:1425:PRO:HD3	1.64	0.79
1:A:990:ILE:HG12	1:A:1160:GLU:HG2	1.64	0.79
1:A:448:PHE:CZ	1:A:456:PHE:HE2	2.03	0.77
1:A:437:ILE:HG23	1:A:458:VAL:CG1	2.15	0.77
1:A:800:ASP:HB3	1:A:803:SER:HB2	1.68	0.76
1:A:24:LEU:O	1:A:26:HIS:CD2	2.39	0.75
1:A:1664:LEU:HD13	1:A:1696:GLN:HA	1.70	0.74
1:A:1026:LEU:O	1:A:1030:ASN:ND2	2.20	0.70
1:A:995:VAL:HB	1:A:1155:LEU:HB2	1.74	0.68
1:B:126:LEU:HD21	1:B:184:LEU:HD22	1.76	0.68
1:A:1424:VAL:HB	1:A:1425:PRO:CD	2.25	0.67
1:A:402:ILE:O	1:A:406:LEU:HB2	1.95	0.67
1:A:368:LEU:HD21	1:A:403:PHE:CE2	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1785:TYR:HB3	1:A:1790:GLN:CB	2.26	0.66
1:A:695:PRO:HB3	1:A:718:ILE:HD11	1.80	0.64
1:A:126:LEU:HD21	1:A:184:LEU:HD22	1.80	0.63
1:A:1111:HIS:HB3	1:A:1112:PRO:HD2	1.81	0.63
1:A:448:PHE:CZ	1:A:456:PHE:CE2	2.86	0.63
1:A:1531:SER:CB	1:A:1532:PRO:HD3	2.18	0.62
1:A:396:ASP:HB3	1:A:488:ILE:HG12	1.80	0.62
1:A:1368:TYR:HA	1:A:1378:GLY:HA2	1.81	0.62
1:A:990:ILE:CG1	1:A:1160:GLU:HG2	2.30	0.60
1:B:513:ILE:CD1	1:B:533:ILE:HG12	2.31	0.60
1:A:1785:TYR:HB3	1:A:1790:GLN:HB3	1.83	0.60
1:A:201:ILE:HG22	1:A:203:LYS:H	1.67	0.60
1:A:552:LYS:O	1:A:554:ILE:HG23	2.02	0.60
1:A:795:ILE:HG12	1:A:1764:LEU:HD22	1.84	0.60
1:B:400:LEU:O	1:B:404:THR:OG1	2.18	0.59
1:A:1029:MET:HE1	1:A:1174:MET:HG2	1.83	0.59
1:A:1337:VAL:O	1:A:1337:VAL:HG12	2.03	0.59
1:A:437:ILE:CG1	1:A:458:VAL:HB	2.25	0.58
1:B:396:ASP:HB2	1:B:488:ILE:HG12	1.85	0.58
1:A:1295:GLY:HA2	1:A:1358:ASN:CG	2.28	0.58
1:A:1773:ILE:O	1:A:1773:ILE:HG22	2.05	0.57
1:B:513:ILE:HD12	1:B:531:LEU:HD21	1.87	0.57
1:A:1069:HIS:HA	1:A:1193:VAL:HB	1.86	0.57
1:A:1464:ILE:HB	1:A:1465:PRO:HD3	1.87	0.57
1:A:1645:ALA:HA	1:A:1663:LEU:HA	1.86	0.56
1:A:1644:ASP:O	1:A:1664:LEU:N	2.36	0.56
1:A:1223:ILE:CG2	1:A:1424:VAL:HG11	2.32	0.56
1:A:1508:ASN:HD22	1:A:1533:VAL:HG12	1.70	0.56
1:A:223:VAL:HG13	1:A:228:SER:HB3	1.87	0.56
1:A:1531:SER:HB2	1:A:1532:PRO:CD	2.23	0.56
1:A:407:LEU:O	1:A:407:LEU:CD2	2.47	0.56
1:A:1664:LEU:HD11	1:A:1697:PHE:H	1.70	0.56
1:A:436:THR:OG1	1:A:437:ILE:HD12	2.07	0.55
1:B:223:VAL:HG13	1:B:228:SER:HB3	1.89	0.55
1:A:458:VAL:HG12	1:A:458:VAL:O	2.06	0.54
1:A:732:VAL:O	1:A:735:LEU:HB3	2.07	0.54
1:A:1329:VAL:HG21	1:A:1340:ASP:OD1	2.07	0.54
1:A:633:ALA:O	1:A:661:HIS:NE2	2.38	0.54
1:A:8:THR:OG1	1:A:9:THR:N	2.41	0.54
1:B:75:SER:HB3	1:B:85:PRO:HB2	1.90	0.54
1:A:1775:TRP:CZ3	1:A:1795:VAL:O	2.62	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:PHE:HA	1:A:398:SER:OG	2.08	0.53
1:A:482:GLY:HA3	1:A:489:MET:HA	1.89	0.53
1:A:1664:LEU:CD1	1:A:1696:GLN:HA	2.37	0.53
1:A:1419:GLU:OE2	1:A:1457:ASN:HB2	2.09	0.53
1:A:281:VAL:HG22	1:A:348:VAL:HB	1.91	0.52
1:A:1145:THR:HB	1:A:1160:GLU:HB2	1.91	0.52
1:A:1393:MET:HE3	1:A:1518:TYR:HD2	1.73	0.52
1:A:75:SER:HB3	1:A:85:PRO:HB2	1.90	0.52
1:A:1423:TRP:CD1	1:A:1430:LEU:HB2	2.44	0.52
1:A:668:THR:OG1	1:A:670:ASN:OD1	2.28	0.51
1:B:281:VAL:HG22	1:B:348:VAL:HB	1.93	0.51
1:A:1248:THR:OG1	1:A:1249:TYR:N	2.44	0.51
1:A:1280:ARG:HG2	1:A:1432:ILE:HG23	1.92	0.51
1:A:600:ILE:HD12	1:A:615:VAL:HG11	1.93	0.50
1:B:251:LYS:O	1:B:254:ASP:HB2	2.11	0.50
1:A:453:ASN:CG	1:A:456:PHE:CD2	2.90	0.50
1:B:482:GLY:HA3	1:B:489:MET:HA	1.94	0.50
1:B:101:HIS:ND1	1:B:102:LEU:O	2.42	0.50
1:B:488:ILE:HG22	1:B:489:MET:HG3	1.94	0.50
1:A:448:PHE:CE2	1:A:456:PHE:CE2	3.00	0.49
1:A:1359:GLN:HG3	1:A:1361:GLY:H	1.76	0.49
1:A:990:ILE:HG23	1:A:1158:VAL:HG13	1.94	0.49
1:A:1177:GLN:HE22	1:A:1555:PRO:HB3	1.77	0.49
1:B:8:THR:OG1	1:B:9:THR:N	2.46	0.49
1:B:466:LEU:HD21	1:B:477:LEU:HD21	1.94	0.49
1:A:488:ILE:HG22	1:A:489:MET:HG3	1.95	0.49
1:A:1457:ASN:OD1	1:A:1483:LEU:HD12	2.13	0.49
1:B:405:HIS:HB3	1:B:410:ALA:HB3	1.94	0.49
1:A:600:ILE:HB	1:A:615:VAL:HG21	1.94	0.48
1:A:1158:VAL:HG12	1:A:1160:GLU:HG3	1.95	0.48
1:A:400:LEU:O	1:A:404:THR:CB	2.61	0.48
1:A:388:LEU:HD23	1:A:413:HIS:HB2	1.95	0.48
1:A:1560:GLY:C	1:A:1601:LEU:HD12	2.38	0.48
1:A:125:THR:HA	1:A:180:THR:HA	1.95	0.48
1:A:453:ASN:CG	1:A:456:PHE:HD2	2.21	0.48
1:A:1295:GLY:HA2	1:A:1358:ASN:ND2	2.28	0.48
1:A:1235:PRO:O	1:A:1248:THR:OG1	2.25	0.48
1:A:1785:TYR:HB3	1:A:1790:GLN:HB2	1.95	0.48
1:A:730:ILE:HA	1:A:733:MET:HE2	1.96	0.48
1:A:1538:PRO:HB3	1:A:1544:MET:HG3	1.94	0.48
1:A:1642:ILE:CD1	1:A:1663:LEU:HD22	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG11	1:B:140:LEU:HD11	1.96	0.48
1:B:283:ILE:HG12	1:B:295:MET:HE2	1.96	0.48
1:A:1414:ASP:O	1:A:1517:ILE:HG12	2.13	0.47
1:A:805:ALA:HA	1:A:1139:ILE:HG21	1.96	0.47
1:A:1560:GLY:O	1:A:1601:LEU:HD12	2.14	0.47
1:A:283:ILE:HG12	1:A:295:MET:HE2	1.96	0.47
1:A:490:VAL:HG11	1:A:533:ILE:HD13	1.97	0.47
1:A:1764:LEU:O	1:A:1764:LEU:HG	2.14	0.47
1:B:388:LEU:HD23	1:B:413:HIS:HB2	1.96	0.47
1:B:390:TYR:HA	1:B:415:VAL:HG11	1.96	0.47
1:B:556:HIS:CE1	1:B:558:GLN:HB2	2.50	0.47
1:A:1663:LEU:O	1:A:1663:LEU:HD12	2.14	0.47
1:A:990:ILE:CD1	1:A:1160:GLU:HG2	2.45	0.46
1:A:1277:MET:HB3	1:A:1301:ILE:HB	1.98	0.46
1:A:1561:GLU:HA	1:A:1600:ASP:O	2.15	0.46
1:A:516:LEU:HB2	1:A:532:PHE:CE1	2.51	0.46
1:A:989:ALA:HB3	1:A:1161:TYR:CZ	2.51	0.46
1:A:1301:ILE:O	1:A:1411:TYR:OH	2.22	0.46
1:A:1737:ILE:HD13	1:A:1770:LEU:HD23	1.97	0.45
1:A:390:TYR:HA	1:A:415:VAL:HG11	1.98	0.45
1:A:448:PHE:HZ	1:A:456:PHE:HE2	1.60	0.45
1:A:794:TYR:HB3	1:A:848:ILE:HD13	1.97	0.45
1:A:1295:GLY:HA2	1:A:1358:ASN:HD21	1.81	0.45
1:A:101:HIS:ND1	1:A:102:LEU:O	2.41	0.45
1:A:620:GLN:HG3	1:A:621:ALA:H	1.81	0.45
1:B:490:VAL:HG11	1:B:533:ILE:HD13	1.98	0.45
1:A:791:LYS:O	1:A:795:ILE:HG13	2.17	0.44
1:A:627:LEU:HB2	1:A:656:PRO:HA	1.99	0.44
1:B:513:ILE:HG21	1:B:578:ILE:HD13	1.99	0.44
1:A:1393:MET:HE3	1:A:1518:TYR:CD2	2.51	0.44
1:A:1226:MET:HB3	1:A:1230:TRP:CZ3	2.52	0.44
1:A:820:THR:HG23	1:A:893:VAL:HG21	1.98	0.44
1:A:1738:TRP:HH2	1:A:1786:PRO:O	2.00	0.44
1:A:912:ASP:CG	1:A:913:GLY:H	2.24	0.43
1:A:1661:ALA:HB2	1:A:1688:PRO:HG2	2.00	0.43
1:B:516:LEU:HB2	1:B:532:PHE:CE1	2.53	0.43
1:B:77:LEU:HD12	1:B:99:THR:HG21	2.00	0.43
1:A:1107:GLU:CB	1:A:1754:PHE:CG	3.01	0.43
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.78	0.43
1:A:874:LEU:HD23	1:A:1135:ILE:HG21	2.01	0.43
1:A:1241:VAL:HB	1:A:1431:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:LEU:HB3	1:A:556:HIS:HE2	1.84	0.43
1:B:205:PHE:CE1	1:B:403:PHE:HB3	2.54	0.43
1:A:614:THR:HG21	1:A:673:VAL:HG11	2.01	0.42
1:B:53:TYR:CE2	1:B:55:TYR:HB2	2.54	0.42
1:B:401:ASP:O	1:B:405:HIS:ND1	2.52	0.42
1:A:216:THR:HB	1:A:219:HIS:CG	2.55	0.42
1:A:1457:ASN:ND2	1:A:1518:TYR:OH	2.52	0.42
1:A:1587:HIS:CG	1:A:1588:PRO:HD2	2.54	0.42
1:A:1663:LEU:HD12	1:A:1663:LEU:C	2.45	0.42
1:B:73:HIS:HD2	1:B:77:LEU:HD21	1.84	0.42
1:A:77:LEU:HD12	1:A:99:THR:HG21	2.01	0.42
1:A:1390:LEU:O	1:A:1394:GLN:HG2	2.20	0.42
1:A:53:TYR:CE2	1:A:55:TYR:HB2	2.54	0.41
1:A:1177:GLN:HB3	1:A:1198:LEU:HB3	2.02	0.41
1:A:1749:ILE:HG23	1:A:1750:ARG:HG3	2.02	0.41
1:B:216:THR:HB	1:B:219:HIS:CG	2.55	0.41
1:A:114:VAL:HG11	1:A:140:LEU:HD11	2.02	0.41
1:A:1467:VAL:HG21	1:A:1497:VAL:HG22	2.03	0.41
1:A:1539:LEU:HB2	1:A:1542:TYR:CD1	2.55	0.41
1:B:213:VAL:HG22	1:B:231:TYR:HB3	2.02	0.41
1:A:437:ILE:HA	1:A:458:VAL:O	2.20	0.41
1:A:1737:ILE:CD1	1:A:1770:LEU:HD23	2.50	0.41
1:A:605:MET:HE2	1:A:612:LEU:HA	2.03	0.41
1:A:866:GLU:H	1:A:869:SER:HG	1.68	0.41
1:A:1385:ALA:HA	1:A:1568:SER:HA	2.02	0.41
1:A:187:LEU:HD22	1:A:524:PRO:HA	2.02	0.41
1:A:651:PRO:HD2	1:A:654:MET:HB2	2.03	0.40
1:A:1724:ALA:HB3	1:A:1749:ILE:HG22	2.03	0.40
1:B:112:ILE:HG21	1:B:115:GLN:HB2	2.03	0.40
1:A:843:MET:HE2	1:A:843:MET:HB2	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1783/1814 (98%)	1641 (92%)	140 (8%)	2 (0%)	48	83
1	B	583/1814 (32%)	547 (94%)	35 (6%)	1 (0%)	43	77
All	All	2366/3628 (65%)	2188 (92%)	175 (7%)	3 (0%)	48	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	ILE
1	B	488	ILE
1	A	1517	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	1527/1562 (98%)	1509 (99%)	18 (1%)	63	75
1	B	499/1562 (32%)	496 (99%)	3 (1%)	78	82
All	All	2026/3124 (65%)	2005 (99%)	21 (1%)	68	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	PHE
1	A	406	LEU
1	A	458	VAL
1	A	572	PHE
1	A	751	LEU
1	A	770	VAL
1	A	775	LEU
1	A	792	ARG
1	A	873	LEU
1	A	1106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1280	ARG
1	A	1326	SER
1	A	1427	ARG
1	A	1458	PHE
1	A	1517	ILE
1	A	1518	TYR
1	A	1547	ILE
1	A	1764	LEU
1	B	254	ASP
1	B	393	PHE
1	B	572	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	73	HIS
1	A	131	ASN
1	A	150	HIS
1	A	211	GLN
1	A	243	HIS
1	A	639	HIS
1	A	702	GLN
1	A	957	GLN
1	A	1059	ASN
1	A	1089	GLN
1	A	1177	GLN
1	A	1184	GLN
1	A	1187	HIS
1	A	1325	GLN
1	A	1359	GLN
1	A	1440	ASN
1	A	1457	ASN
1	A	1508	ASN
1	A	1618	HIS
1	A	1651	ASN
1	B	26	HIS
1	B	73	HIS
1	B	80	ASN
1	B	150	HIS
1	B	211	GLN

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PNS	A	1901	1	0,3,21	-	-	0,3,29	-	-
2	PNS	A	1902	1	0,3,21	-	-	0,3,29	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	1789/1814 (98%)	0.74	216 (12%)	8 16	238, 340, 430, 496	0
1	B	585/1814 (32%)	0.73	74 (12%)	8 15	244, 332, 405, 439	0
All	All	2374/3628 (65%)	0.74	290 (12%)	8 16	238, 337, 424, 496	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	725	ARG	11.0
1	A	390	TYR	8.8
1	B	536	GLU	7.6
1	A	722	PHE	7.5
1	B	486	CYS	6.8
1	A	657	THR	6.7
1	A	391	SER	6.5
1	A	939	TYR	6.4
1	A	942	PHE	6.3
1	A	400	LEU	6.2
1	A	658	TYR	6.2
1	B	485	GLU	6.1
1	A	583	ARG	6.0
1	A	399	ALA	6.0
1	A	396	ASP	6.0
1	A	486	CYS	5.7
1	A	1053	LEU	5.6
1	B	488	ILE	5.4
1	A	397	GLY	5.4
1	A	1213	ASP	5.1
1	A	265	ASP	5.1
1	A	439	TYR	5.0
1	A	1421	PHE	5.0
1	A	389	VAL	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	326	PRO	4.9
1	A	938	THR	4.9
1	A	485	GLU	4.9
1	B	131	ASN	4.8
1	A	694	ALA	4.8
1	A	627	LEU	4.8
1	A	403	PHE	4.7
1	B	400	LEU	4.7
1	A	481	TYR	4.6
1	A	401	ASP	4.6
1	A	337	PRO	4.6
1	A	1544	MET	4.5
1	A	488	ILE	4.5
1	A	398	SER	4.4
1	B	564	TYR	4.4
1	A	720	ASP	4.3
1	B	568	ASP	4.2
1	A	1357	VAL	4.2
1	A	463	GLY	4.2
1	A	1108	GLY	4.2
1	A	937	LYS	4.2
1	A	1121	GLN	4.2
1	A	1240	LEU	4.2
1	B	347	TYR	4.1
1	B	481	TYR	4.1
1	A	266	MET	4.1
1	A	715	GLN	4.0
1	A	1559	PRO	3.9
1	A	872	SER	3.9
1	B	396	ASP	3.9
1	A	324	HIS	3.9
1	A	726	GLY	3.9
1	A	205	PHE	3.9
1	A	116	GLU	3.9
1	A	533	ILE	3.8
1	A	1	MET	3.8
1	A	675	ARG	3.7
1	A	347	TYR	3.7
1	A	1107	GLU	3.7
1	A	936	GLU	3.7
1	B	252	PRO	3.6
1	B	412	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1545	TYR	3.6
1	A	274	MET	3.6
1	B	368	LEU	3.6
1	A	267	ILE	3.6
1	A	1285	MET	3.6
1	A	490	VAL	3.5
1	B	371	PHE	3.5
1	A	402	ILE	3.5
1	A	615	VAL	3.5
1	A	727	GLY	3.5
1	A	775	LEU	3.4
1	A	1644	ASP	3.4
1	A	642	LEU	3.4
1	A	1613	LEU	3.4
1	A	559	THR	3.4
1	B	566	THR	3.4
1	B	369	VAL	3.3
1	A	271	LEU	3.3
1	B	487	THR	3.3
1	A	1134	HIS	3.3
1	B	538	LEU	3.3
1	B	267	ILE	3.2
1	B	222	VAL	3.2
1	A	335	ASN	3.2
1	A	1160	GLU	3.2
1	A	1047	HIS	3.2
1	B	403	PHE	3.2
1	A	1241	VAL	3.2
1	A	1106	ARG	3.2
1	A	927	LEU	3.1
1	A	303	ILE	3.1
1	B	303	ILE	3.1
1	B	533	ILE	3.1
1	A	484	THR	3.1
1	A	464	ASP	3.1
1	A	270	ILE	3.1
1	A	371	PHE	3.1
1	A	1125	GLU	3.1
1	A	926	LEU	3.0
1	A	734	GLN	3.0
1	A	466	LEU	3.0
1	A	483	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1645	ALA	3.0
1	A	1486	GLY	3.0
1	A	1046	GLN	3.0
1	A	1772	ARG	3.0
1	A	412	LEU	3.0
1	A	338	HIS	3.0
1	A	656	PRO	3.0
1	A	1488	ALA	3.0
1	A	1338	VAL	3.0
1	A	711	LEU	2.9
1	B	372	CYS	2.9
1	B	280	TYR	2.9
1	A	1733	THR	2.9
1	A	207	GLN	2.9
1	B	205	PHE	2.9
1	A	617	ALA	2.9
1	A	693	VAL	2.9
1	A	628	VAL	2.9
1	B	404	THR	2.9
1	A	940	LYS	2.9
1	B	340	ASN	2.9
1	A	713	ILE	2.9
1	A	113	LEU	2.9
1	A	300	SER	2.8
1	A	1601	LEU	2.8
1	B	293	ALA	2.8
1	A	724	GLU	2.8
1	B	544	ASN	2.8
1	A	1564	ILE	2.8
1	A	835	GLU	2.8
1	A	1340	ASP	2.8
1	A	1702	ASN	2.8
1	A	1513	THR	2.8
1	B	290	GLU	2.8
1	B	399	ALA	2.8
1	A	513	ILE	2.7
1	A	670	ASN	2.7
1	B	489	MET	2.7
1	A	1692	VAL	2.7
1	B	141	PHE	2.7
1	A	1050	THR	2.7
1	A	1413	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	590	ILE	2.7
1	A	1378	GLY	2.7
1	B	277	GLY	2.6
1	B	19	ARG	2.6
1	A	159	THR	2.6
1	B	417	SER	2.6
1	A	908	HIS	2.6
1	A	262	LYS	2.6
1	A	972	ALA	2.6
1	A	246	ARG	2.6
1	B	274	MET	2.6
1	A	368	LEU	2.6
1	A	716	MET	2.6
1	B	262	LYS	2.6
1	A	867	GLU	2.6
1	A	973	VAL	2.6
1	A	626	TYR	2.6
1	A	209	PHE	2.5
1	A	618	LYS	2.5
1	B	338	HIS	2.5
1	B	289	GLY	2.5
1	A	550	ALA	2.5
1	B	546	PRO	2.5
1	A	70	ILE	2.5
1	A	406	LEU	2.5
1	A	1339	LEU	2.5
1	A	1052	GLU	2.5
1	A	30	ILE	2.5
1	B	339	VAL	2.5
1	A	1141	LYS	2.5
1	B	335	ASN	2.5
1	A	1215	ALA	2.5
1	B	297	ALA	2.5
1	A	551	GLU	2.5
1	A	1635	LYS	2.5
1	B	16	LYS	2.5
1	B	288	PRO	2.5
1	A	323	VAL	2.5
1	A	1677	LEU	2.5
1	A	1646	VAL	2.5
1	B	535	GLY	2.5
1	A	672	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1633	ARG	2.4
1	A	393	PHE	2.4
1	A	714	PRO	2.4
1	B	322	ASP	2.4
1	B	294	TYR	2.4
1	A	1431	VAL	2.4
1	B	17	VAL	2.4
1	A	487	THR	2.4
1	B	23	SER	2.4
1	B	313	LYS	2.4
1	A	1054	LEU	2.4
1	B	375	TYR	2.4
1	A	13	LYS	2.4
1	B	115	GLN	2.4
1	A	1066	SER	2.4
1	B	286	ASP	2.4
1	B	483	PRO	2.3
1	A	1492	GLU	2.3
1	A	280	TYR	2.3
1	A	73	HIS	2.3
1	B	513	ILE	2.3
1	A	591	ARG	2.3
1	A	269	SER	2.3
1	A	941	SER	2.3
1	A	74	PRO	2.3
1	B	402	ILE	2.3
1	A	1359	GLN	2.3
1	A	514	LEU	2.3
1	A	806	TYR	2.3
1	B	390	TYR	2.3
1	A	6	PHE	2.3
1	A	552	LYS	2.3
1	A	822	GLN	2.3
1	A	361	VAL	2.3
1	B	406	LEU	2.3
1	A	653	TYR	2.2
1	A	1238	THR	2.2
1	A	844	ARG	2.2
1	A	1057	PHE	2.2
1	B	118	ILE	2.2
1	A	1773	ILE	2.2
1	B	71	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	346	VAL	2.2
1	A	616	LEU	2.2
1	A	1589	LEU	2.2
1	A	369	VAL	2.2
1	A	544	ASN	2.2
1	A	565	ARG	2.2
1	A	1327	PRO	2.2
1	A	144	GLU	2.2
1	A	914	LEU	2.2
1	A	1631	GLU	2.2
1	A	861	VAL	2.2
1	A	637	ILE	2.2
1	B	263	SER	2.2
1	A	538	LEU	2.2
1	A	541	GLY	2.2
1	A	208	LEU	2.2
1	A	745	SER	2.2
1	A	794	TYR	2.2
1	A	1510	TYR	2.2
1	B	261	ASP	2.1
1	A	1370	SER	2.1
1	A	784	TYR	2.1
1	B	490	VAL	2.1
1	A	155	PRO	2.1
1	A	1678	LEU	2.1
1	A	1518	TYR	2.1
1	A	1701	ALA	2.1
1	A	829	GLN	2.1
1	A	377	PRO	2.1
1	A	665	PHE	2.1
1	A	1083	LYS	2.1
1	A	1143	ASP	2.1
1	A	420	LYS	2.1
1	A	960	ALA	2.1
1	A	813	ASN	2.1
1	A	161	GLY	2.1
1	A	798	GLN	2.1
1	A	1221	LYS	2.1
1	A	580	PHE	2.1
1	A	1433	LEU	2.0
1	A	1298	TYR	2.0
1	A	482	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1420	ILE	2.0
1	B	321	ILE	2.0
1	A	489	MET	2.0
1	B	553	PHE	2.0
1	A	52	ALA	2.0
1	A	407	LEU	2.0
1	A	1742	LEU	2.0
1	B	130	TYR	2.0
1	B	537	GLY	2.0
1	A	86	VAL	2.0
1	A	673	VAL	2.0
1	A	735	LEU	2.0
1	A	866	GLU	2.0
1	B	144	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PNS	A	1901	4/22	0.32	0.33	331,348,366,394	0
2	PNS	A	1902	4/22	0.68	0.17	374,377,381,388	0

6.5 Other polymers [i](#)

There are no such residues in this entry.