



Full wwPDB X-ray Structure Validation Report

Jun 29, 2014 – 10:50 PM EDT

PDB ID : 3ML9
Title : Discovery of the Highly Potent PI3K/mTOR Dual Inhibitor PF-04691502
through Structure Based Drug Design
Authors : Knighton, D.R.
Deposited on : 2010-04-16
Resolution : 2.55 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

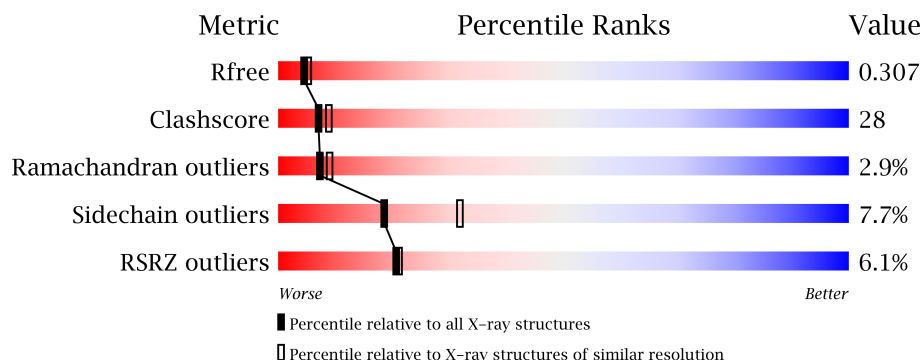
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.55 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6896 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

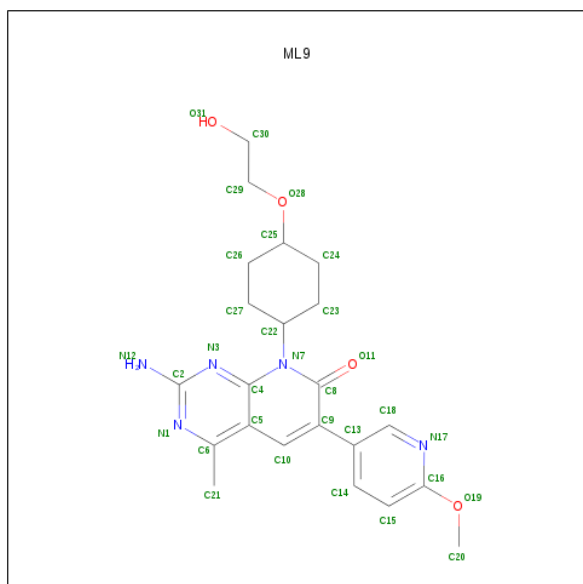
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	847	Total	C	N	O	S	0	0	0
			6864	4413	1170	1246	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	ARG	GLN	CONFLICT	UNP P48736

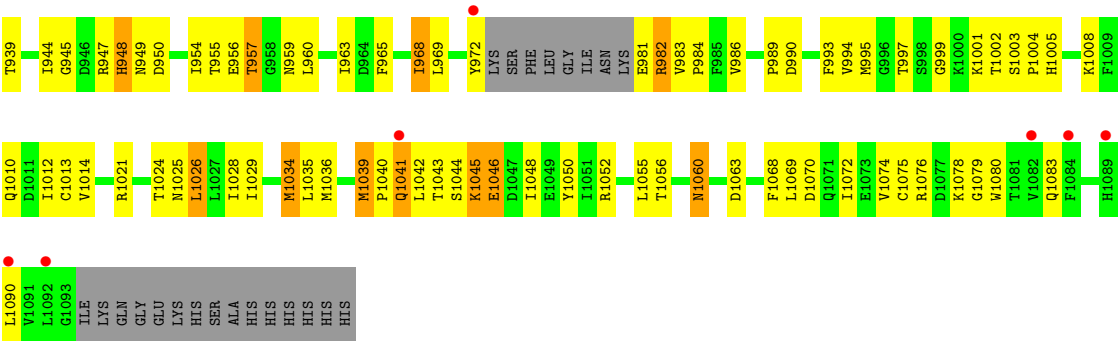
- Molecule 2 is 2-AMINO-8-[TRANS-4-(2-HYDROXYETHOXY)CYCLOHEXYL]-6-(6-METHOXYPYRIDIN-3-YL)-4-METHYLPYRIDO[2,3-D]PYRIMIDIN-7(8H)-ONE (three-letter code: ML9) (formula: C₂₂H₂₇N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	22	5	4		

- Molecule 3 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.93Å 67.29Å 106.84Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	44.79 – 2.55 44.79 – 2.52	Depositor EDS
% Data completeness (in resolution range)	95.9 (44.79-2.55) 95.3 (44.79-2.52)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.51Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.242 , 0.298 0.251 , 0.307	Depositor DCC
R_{free} test set	1625 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34166 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ML9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/7012	0.54	0/9487

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6864	0	6913	394	0
2	A	31	0	27	4	0
3	A	1	0	0	0	0
All	All	6896	0	6940	394	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (394) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:568:THR:HG23	1:A:571:ASP:H	1.17	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.47	0.96
1:A:523:TYR:HB2	1:A:525:HIS:HB3	1.48	0.94
1:A:887:THR:HG22	1:A:889:ALA:H	1.31	0.94
1:A:807:LYS:HD2	1:A:807:LYS:H	1.34	0.93
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.53	0.91
1:A:197:ALA:HA	1:A:689:LYS:HE3	1.53	0.90
1:A:149:ALA:HA	1:A:152:ARG:HD3	1.56	0.86
1:A:320:LYS:H	1:A:320:LYS:HD2	1.39	0.85
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.43	0.84
1:A:359:ARG:HH11	1:A:359:ARG:HB2	1.42	0.83
1:A:523:TYR:HB2	1:A:525:HIS:CB	2.09	0.83
1:A:370:ILE:HD13	1:A:372:VAL:H	1.43	0.82
1:A:524:CYS:N	1:A:525:HIS:HB2	1.95	0.82
1:A:210:TYR:HA	1:A:213:LYS:HD3	1.63	0.81
1:A:968:ILE:HD13	1:A:968:ILE:H	1.47	0.80
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.46	0.80
1:A:370:ILE:CD1	1:A:372:VAL:H	1.96	0.78
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.65	0.78
1:A:369:ASP:OD1	1:A:515:SER:HB3	1.84	0.77
1:A:359:ARG:HB2	1:A:359:ARG:NH1	2.00	0.77
1:A:887:THR:HG22	1:A:889:ALA:N	1.98	0.77
1:A:939:THR:OG1	1:A:945:GLY:HA2	1.85	0.77
1:A:221:PHE:HE2	1:A:234:LYS:HG2	1.50	0.76
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.66	0.75
1:A:1040:PRO:O	1:A:1041:GLN:HB2	1.86	0.75
1:A:496:SER:HB2	1:A:1044:SER:HA	1.68	0.75
1:A:882:VAL:HG23	2:A:9999:ML9:H21	1.67	0.75
1:A:763:VAL:HA	1:A:766:GLN:HE22	1.50	0.74
1:A:990:ASP:O	1:A:994:VAL:HG23	1.88	0.74
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.70	0.73
1:A:749:ILE:HG21	1:A:803:VAL:HG21	1.69	0.73
1:A:207:LEU:HD11	1:A:211:LEU:HB2	1.71	0.73
1:A:763:VAL:HA	1:A:766:GLN:NE2	2.05	0.72
1:A:995:MET:O	1:A:1005:HIS:HB2	1.90	0.72
1:A:732:PHE:O	1:A:736:VAL:HG23	1.91	0.71
1:A:548:PRO:HD2	1:A:551:LEU:HD12	1.73	0.71
1:A:165:VAL:O	1:A:165:VAL:HG12	1.91	0.71
1:A:997:THR:HG21	1:A:1076:ARG:NH1	2.06	0.71
1:A:236:SER:HB3	1:A:239:ASP:OD1	1.90	0.70
1:A:1056:THR:HG23	1:A:1056:THR:O	1.90	0.70
1:A:149:ALA:HB1	1:A:152:ARG:NH1	2.06	0.70
1:A:558:ILE:O	1:A:561:THR:HG22	1.89	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:530:PRO:O	1:A:531:LYS:HB2	1.91	0.70
1:A:530:PRO:O	1:A:531:LYS:CB	2.39	0.70
1:A:568:THR:HG23	1:A:571:ASP:N	2.01	0.70
1:A:935:TYR:O	1:A:939:THR:HG22	1.92	0.69
1:A:523:TYR:N	1:A:523:TYR:CD1	2.56	0.69
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.09	0.68
1:A:981:GLU:OE1	1:A:1078:LYS:HE3	1.94	0.67
1:A:804:MET:CE	1:A:812:TRP:HB2	2.25	0.67
1:A:207:LEU:CD1	1:A:211:LEU:HB2	2.25	0.67
1:A:864:LEU:O	1:A:865:LEU:HD12	1.94	0.67
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.58	0.66
1:A:355:TRP:CD2	1:A:530:PRO:HG2	2.30	0.66
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.75	0.66
1:A:202:VAL:HG13	1:A:285:THR:HG21	1.77	0.66
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.30	0.66
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.30	0.66
1:A:524:CYS:CB	1:A:525:HIS:HB2	2.26	0.66
1:A:972:TYR:O	1:A:1042:LEU:HD21	1.96	0.66
1:A:466:LEU:HD11	1:A:476:ARG:CD	2.27	0.65
1:A:767:LEU:O	1:A:771:LEU:HG	1.97	0.65
1:A:547:MET:HG2	1:A:552:ARG:NH1	2.11	0.65
1:A:153:GLN:O	1:A:156:ALA:HB3	1.97	0.64
1:A:355:TRP:CE3	1:A:530:PRO:HG2	2.32	0.64
1:A:1005:HIS:CE1	1:A:1008:LYS:HZ1	2.16	0.64
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.28	0.64
1:A:767:LEU:CD1	1:A:803:VAL:HG23	2.28	0.64
1:A:1055:LEU:O	1:A:1056:THR:HG22	1.97	0.64
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.80	0.64
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.10	0.64
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.79	0.63
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.79	0.63
1:A:497:PHE:H	1:A:1043:THR:HG21	1.64	0.63
1:A:235:VAL:HG13	1:A:239:ASP:OD2	1.98	0.63
1:A:524:CYS:SG	1:A:525:HIS:HB2	2.39	0.63
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.80	0.63
1:A:306:VAL:HG21	1:A:821:THR:HG21	1.81	0.63
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.46	0.63
1:A:955:THR:C	1:A:957:THR:H	2.00	0.63
1:A:305:VAL:HG12	1:A:307:LEU:H	1.64	0.63
1:A:320:LYS:CD	1:A:320:LYS:H	2.04	0.62
1:A:1024:THR:O	1:A:1028:ILE:HD12	1.99	0.62
1:A:524:CYS:CA	1:A:525:HIS:HB2	2.28	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:833:LYS:NZ	2:A:9999:ML9:H15	2.15	0.62
1:A:555:LEU:HD13	1:A:574:LEU:CD1	2.30	0.62
1:A:775:GLN:HE22	1:A:795:ALA:HA	1.64	0.62
1:A:273:ARG:O	1:A:305:VAL:HG13	2.00	0.61
1:A:697:TRP:CZ3	1:A:872:THR:HG22	2.35	0.61
1:A:287:ILE:HD12	1:A:288:LYS:N	2.14	0.61
1:A:657:LEU:HG	1:A:691:ILE:HD13	1.82	0.61
1:A:782:SER:O	1:A:783:PHE:HB3	2.00	0.61
1:A:173:LEU:O	1:A:177:ARG:HG3	2.00	0.61
1:A:900:GLY:HA2	1:A:902:PHE:CZ	2.35	0.61
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.82	0.61
1:A:1043:THR:O	1:A:1045:LYS:N	2.31	0.61
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.35	0.61
1:A:1069:LEU:HA	1:A:1072:ILE:HD12	1.82	0.61
1:A:910:TRP:HE3	1:A:911:LEU:HD23	1.66	0.61
1:A:568:THR:HG22	1:A:571:ASP:CG	2.21	0.61
1:A:370:ILE:HD12	1:A:372:VAL:O	2.00	0.60
1:A:760:SER:OG	1:A:763:VAL:HG23	2.00	0.60
1:A:833:LYS:HZ1	2:A:9999:ML9:H15	1.65	0.60
1:A:472:ARG:O	1:A:473:PHE:HB2	1.99	0.60
1:A:561:THR:HG23	1:A:591:LYS:NZ	2.16	0.60
1:A:774:LEU:C	1:A:776:ASN:H	2.05	0.60
1:A:162:VAL:HG21	1:A:718:GLU:OE1	2.01	0.60
1:A:955:THR:OG1	1:A:957:THR:HG23	2.01	0.60
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.83	0.59
1:A:1072:ILE:O	1:A:1075:CYS:HB2	2.02	0.59
1:A:498:ASN:HD21	1:A:500:ASP:HB2	1.67	0.59
1:A:214:LYS:NZ	1:A:214:LYS:HB3	2.17	0.59
1:A:221:PHE:CE2	1:A:234:LYS:HG2	2.36	0.59
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.03	0.59
1:A:947:ARG:NH1	1:A:948:HIS:NE2	2.51	0.59
1:A:497:PHE:N	1:A:1043:THR:HG21	2.18	0.58
1:A:690:ARG:NH1	1:A:789:PRO:HG2	2.17	0.58
1:A:801:CYS:HA	1:A:812:TRP:O	2.03	0.58
1:A:181:VAL:HG12	1:A:185:MET:CE	2.32	0.58
1:A:352:VAL:O	1:A:527:ILE:HA	2.03	0.58
1:A:147:SER:HB2	1:A:319:ARG:HH22	1.67	0.58
1:A:689:LYS:HG2	1:A:728:MET:SD	2.43	0.58
1:A:745:VAL:HG12	1:A:749:ILE:HD13	1.86	0.58
1:A:250:THR:O	1:A:250:THR:HG22	2.04	0.58
1:A:207:LEU:HD13	1:A:208:PRO:HD2	1.84	0.58
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:807:LYS:HD2	1:A:807:LYS:N	2.13	0.58
1:A:935:TYR:O	1:A:939:THR:CG2	2.51	0.58
1:A:524:CYS:HB2	1:A:525:HIS:CA	2.34	0.57
1:A:568:THR:CG2	1:A:571:ASP:H	2.06	0.57
1:A:701:SER:O	1:A:705:GLN:HG2	2.04	0.57
1:A:531:LYS:O	1:A:531:LYS:HG2	2.04	0.57
1:A:910:TRP:CE3	1:A:911:LEU:HD23	2.40	0.57
1:A:758:ASP:OD1	1:A:758:ASP:N	2.37	0.57
1:A:223:VAL:HB	1:A:304:HIS:ND1	2.19	0.57
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.39	0.57
1:A:947:ARG:NH2	1:A:963:ILE:O	2.38	0.57
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.05	0.57
1:A:523:TYR:HB2	1:A:525:HIS:CG	2.40	0.56
1:A:230:SER:O	1:A:231:GLN:HB2	2.05	0.56
1:A:562:ASP:OD2	1:A:1052:ARG:NH1	2.37	0.56
1:A:281:LEU:HD12	1:A:290:PHE:CD2	2.40	0.56
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.20	0.56
1:A:548:PRO:CD	1:A:551:LEU:HD12	2.36	0.56
1:A:921:PHE:O	1:A:925:VAL:HG23	2.06	0.56
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.70	0.56
1:A:816:LYS:NZ	1:A:816:LYS:HB2	2.21	0.56
1:A:1024:THR:HG22	1:A:1028:ILE:HD12	1.87	0.56
1:A:524:CYS:HB2	1:A:525:HIS:HA	1.87	0.55
1:A:171:ASP:CG	1:A:472:ARG:HH12	2.09	0.55
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.88	0.55
1:A:370:ILE:HD13	1:A:371:PRO:N	2.21	0.55
1:A:1044:SER:O	1:A:1045:LYS:CB	2.54	0.55
1:A:833:LYS:HE3	1:A:836:ASP:OD2	2.07	0.55
1:A:768:LYS:O	1:A:772:GLU:HG3	2.07	0.55
1:A:761:SER:HA	1:A:764:ILE:HD12	1.88	0.55
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.36	0.55
1:A:652:GLU:OE1	1:A:654:ASP:HB3	2.07	0.54
1:A:244:ILE:O	1:A:244:ILE:HG22	2.07	0.54
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.73	0.54
1:A:165:VAL:O	1:A:165:VAL:CG1	2.56	0.54
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.23	0.54
1:A:900:GLY:HA2	1:A:902:PHE:CE2	2.43	0.54
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.38	0.54
1:A:841:ASP:O	1:A:845:LEU:HD22	2.08	0.54
1:A:900:GLY:C	1:A:902:PHE:H	2.11	0.54
1:A:162:VAL:HG12	1:A:714:ALA:HB1	1.90	0.53
1:A:812:TRP:O	1:A:812:TRP:CD1	2.62	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:463:TYR:CD2	1:A:487:ILE:HD11	2.43	0.53
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.23	0.53
1:A:947:ARG:NH1	1:A:968:ILE:HG23	2.23	0.53
1:A:896:VAL:HG13	1:A:901:ALA:HB3	1.91	0.53
1:A:498:ASN:ND2	1:A:500:ASP:H	2.07	0.53
1:A:568:THR:HG22	1:A:571:ASP:OD2	2.09	0.53
1:A:273:ARG:HB3	1:A:306:VAL:HG12	1.89	0.53
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.43	0.53
1:A:319:ARG:HG3	1:A:319:ARG:NH1	2.23	0.53
1:A:899:THR:HG22	1:A:901:ALA:H	1.74	0.53
1:A:182:THR:N	1:A:183:PRO:HD2	2.24	0.53
1:A:529:LEU:HD12	1:A:530:PRO:HD2	1.91	0.53
1:A:272:LEU:HB3	1:A:305:VAL:CG1	2.38	0.53
1:A:864:LEU:C	1:A:865:LEU:HD12	2.28	0.53
1:A:840:GLN:HG2	1:A:1039:MET:HE2	1.91	0.52
1:A:657:LEU:HG	1:A:691:ILE:CD1	2.39	0.52
1:A:739:ILE:O	1:A:743:GLN:HG3	2.09	0.52
1:A:507:ASN:OD1	1:A:508:PRO:HD2	2.09	0.52
1:A:181:VAL:O	1:A:185:MET:HE2	2.09	0.52
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.45	0.52
1:A:748:ASP:HB3	1:A:770:LYS:NZ	2.24	0.52
1:A:302:GLU:HG3	1:A:304:HIS:NE2	2.25	0.52
1:A:351:THR:HA	1:A:526:PRO:HG2	1.91	0.52
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.39	0.52
1:A:364:LYS:HE2	1:A:411:ASN:O	2.09	0.52
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.39	0.52
1:A:907:LEU:O	1:A:911:LEU:HG	2.10	0.52
1:A:288:LYS:HG3	1:A:289:ASN:OD1	2.09	0.52
1:A:366:ARG:NH1	1:A:479:GLU:OE2	2.43	0.52
1:A:273:ARG:HB3	1:A:306:VAL:CG1	2.40	0.52
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.45	0.52
1:A:968:ILE:HG12	1:A:969:LEU:N	2.25	0.52
1:A:516:ILE:HG13	1:A:517:SER:N	2.25	0.51
1:A:843:LEU:HD23	1:A:1034:MET:HG2	1.92	0.51
1:A:498:ASN:HD22	1:A:500:ASP:H	1.58	0.51
1:A:561:THR:HG23	1:A:591:LYS:HZ2	1.75	0.51
1:A:799:GLU:HG3	1:A:800:LYS:HG3	1.93	0.51
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.92	0.51
1:A:614:ARG:HG2	1:A:614:ARG:O	2.10	0.51
1:A:629:GLN:HA	1:A:1029:ILE:HD13	1.93	0.51
1:A:196:TYR:O	1:A:689:LYS:HD2	2.11	0.51
1:A:184:ARG:O	1:A:188:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:LEU:HD11	1:A:211:LEU:CB	2.38	0.51
1:A:198:MET:CE	1:A:282:VAL:HG11	2.41	0.51
1:A:531:LYS:O	1:A:531:LYS:CG	2.55	0.51
1:A:242:GLY:O	1:A:245:LEU:HB2	2.11	0.50
1:A:635:PHE:O	1:A:641:ARG:HD2	2.11	0.50
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.93	0.50
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.93	0.50
1:A:823:LEU:HD12	1:A:824:SER:H	1.77	0.50
1:A:947:ARG:CZ	1:A:968:ILE:HD12	2.40	0.50
1:A:152:ARG:HB2	1:A:152:ARG:HH11	1.77	0.50
1:A:282:VAL:HG12	1:A:283:GLY:N	2.26	0.50
1:A:202:VAL:HG12	1:A:203:THR:H	1.75	0.50
1:A:315:LEU:O	1:A:727:ALA:HB2	2.11	0.50
1:A:801:CYS:HB3	1:A:813:LEU:HD23	1.93	0.50
1:A:202:VAL:HG12	1:A:203:THR:N	2.27	0.49
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.42	0.49
1:A:177:ARG:HG2	1:A:715:VAL:HG13	1.93	0.49
1:A:272:LEU:CB	1:A:305:VAL:HG11	2.41	0.49
1:A:319:ARG:HG3	1:A:319:ARG:HH11	1.77	0.49
1:A:466:LEU:CD1	1:A:476:ARG:HH11	2.26	0.49
1:A:523:TYR:C	1:A:525:HIS:CB	2.80	0.49
1:A:774:LEU:O	1:A:776:ASN:N	2.46	0.49
1:A:547:MET:O	1:A:548:PRO:O	2.31	0.49
1:A:955:THR:C	1:A:957:THR:N	2.66	0.49
1:A:797:ALA:O	1:A:798:ILE:C	2.51	0.49
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.12	0.49
1:A:558:ILE:HG21	1:A:575:LEU:CD2	2.32	0.49
1:A:320:LYS:HD2	1:A:320:LYS:N	2.19	0.48
1:A:282:VAL:HG12	1:A:283:GLY:H	1.78	0.48
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.46	0.48
1:A:1025:ASN:O	1:A:1029:ILE:HG22	2.13	0.48
1:A:241:PRO:HD3	1:A:285:THR:O	2.14	0.48
1:A:250:THR:O	1:A:251:LYS:HB3	2.11	0.48
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.29	0.48
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.95	0.48
1:A:1056:THR:CG2	1:A:1056:THR:O	2.62	0.48
1:A:524:CYS:N	1:A:525:HIS:CB	2.72	0.48
1:A:874:ASP:O	1:A:876:ILE:HG22	2.12	0.48
1:A:949:ASN:N	1:A:1083:GLN:NE2	2.62	0.48
1:A:800:LYS:O	1:A:802:LYS:HG3	2.14	0.48
1:A:207:LEU:HD13	1:A:208:PRO:CD	2.44	0.47
1:A:380:THR:O	1:A:435:CYS:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:TYR:C	1:A:525:HIS:HB3	2.34	0.47
1:A:307:LEU:C	1:A:307:LEU:HD23	2.35	0.47
1:A:180:LEU:C	1:A:183:PRO:HD2	2.34	0.47
1:A:147:SER:HB2	1:A:319:ARG:NH2	2.29	0.47
1:A:925:VAL:O	1:A:929:VAL:HG23	2.15	0.47
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.80	0.47
1:A:787:TYR:CZ	1:A:880:GLU:HB2	2.50	0.47
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.44	0.47
1:A:565:ASN:HB2	1:A:1052:ARG:HH12	1.80	0.47
1:A:731:ASP:O	1:A:735:GLN:HG3	2.15	0.47
1:A:812:TRP:O	1:A:812:TRP:HD1	1.95	0.47
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.13	0.47
1:A:149:ALA:HA	1:A:152:ARG:CD	2.37	0.47
1:A:753:SER:HB2	1:A:809:LYS:HE3	1.96	0.47
1:A:607:THR:O	1:A:610:LEU:HB2	2.14	0.47
1:A:245:LEU:O	1:A:249:PHE:HB2	2.15	0.46
1:A:563:PRO:HD3	1:A:1025:ASN:OD1	2.15	0.46
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.50	0.46
1:A:702:GLU:OE2	1:A:839:ARG:HD3	2.15	0.46
1:A:558:ILE:CG2	1:A:575:LEU:HD21	2.32	0.46
1:A:641:ARG:NH1	1:A:670:GLU:OE1	2.40	0.46
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.13	0.46
1:A:546:GLU:HG3	1:A:547:MET:H	1.80	0.46
1:A:174:GLU:O	1:A:178:ARG:HD2	2.16	0.46
1:A:275:CYS:SG	1:A:304:HIS:HB3	2.56	0.46
1:A:944:ILE:HD12	1:A:965:PHE:HD2	1.80	0.46
1:A:667:VAL:O	1:A:712:ARG:NH1	2.49	0.46
1:A:181:VAL:HG12	1:A:185:MET:HE1	1.98	0.46
1:A:145:GLU:O	1:A:148:GLN:N	2.50	0.45
1:A:394:LEU:HB3	1:A:418:ILE:CD1	2.46	0.45
1:A:784:ARG:NH1	1:A:789:PRO:O	2.49	0.45
1:A:1060:ASN:ND2	1:A:1060:ASN:H	2.14	0.45
1:A:309:THR:HG23	1:A:310:PRO:HD2	1.99	0.45
1:A:778:GLN:O	1:A:779:LEU:C	2.53	0.45
1:A:180:LEU:O	1:A:183:PRO:HD2	2.17	0.45
1:A:248:PHE:C	1:A:250:THR:H	2.20	0.45
1:A:291:GLN:CA	1:A:291:GLN:HE21	2.13	0.45
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.16	0.45
1:A:1002:THR:HG22	1:A:1003:SER:N	2.31	0.45
1:A:198:MET:HE3	1:A:282:VAL:HG11	1.99	0.45
1:A:319:ARG:CG	1:A:319:ARG:HH11	2.30	0.45
1:A:982:ARG:HB2	1:A:982:ARG:HE	1.62	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144:SER:HB3	1:A:147:SER:OG	2.18	0.44
1:A:246:GLN:NE2	1:A:246:GLN:N	2.66	0.44
1:A:601:GLN:HG3	1:A:602:GLU:N	2.32	0.44
1:A:682:LEU:HD22	1:A:686:LEU:HD11	1.99	0.44
1:A:657:LEU:HD11	1:A:690:ARG:HG2	1.99	0.44
1:A:876:ILE:HG12	1:A:877:GLY:N	2.30	0.44
1:A:1002:THR:CG2	1:A:1003:SER:N	2.79	0.44
1:A:823:LEU:N	1:A:823:LEU:HD12	2.32	0.44
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.52	0.44
1:A:738:VAL:HG11	1:A:783:PHE:CE1	2.52	0.44
1:A:1090:LEU:HA	1:A:1090:LEU:HD12	1.82	0.44
1:A:497:PHE:O	1:A:1043:THR:HG21	2.17	0.44
1:A:280:TYR:HB3	1:A:282:VAL:CG2	2.47	0.44
1:A:394:LEU:N	1:A:394:LEU:HD23	2.33	0.44
1:A:965:PHE:HA	1:A:968:ILE:HD11	1.99	0.44
1:A:862:LEU:HD22	1:A:862:LEU:N	2.33	0.44
1:A:198:MET:O	1:A:199:HIS:C	2.56	0.44
1:A:762:GLN:O	1:A:766:GLN:NE2	2.51	0.44
1:A:939:THR:OG1	1:A:945:GLY:CA	2.63	0.44
1:A:382:PHE:CE2	1:A:398:ARG:HD3	2.53	0.43
1:A:149:ALA:CA	1:A:152:ARG:HD3	2.39	0.43
1:A:617:TRP:CZ3	1:A:626:LEU:HD13	2.53	0.43
1:A:523:TYR:HD1	1:A:523:TYR:H	1.51	0.43
1:A:739:ILE:HD12	1:A:740:GLU:N	2.33	0.43
1:A:945:GLY:O	1:A:986:VAL:HG23	2.19	0.43
1:A:1045:LYS:HB3	1:A:1046:GLU:OE1	2.17	0.43
1:A:1060:ASN:ND2	1:A:1063:ASP:OD2	2.52	0.43
1:A:226:ARG:HD2	1:A:226:ARG:HA	1.80	0.43
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.74	0.43
1:A:647:LYS:HA	1:A:647:LYS:HD2	1.61	0.43
1:A:900:GLY:C	1:A:902:PHE:N	2.72	0.43
1:A:824:SER:OG	1:A:825:ASN:N	2.52	0.43
1:A:514:MET:HG3	1:A:515:SER:N	2.34	0.43
1:A:750:LYS:HE2	1:A:808:LYS:HB3	2.00	0.43
1:A:770:LYS:O	1:A:773:ASN:HB2	2.19	0.43
1:A:775:GLN:HA	1:A:775:GLN:OE1	2.18	0.43
1:A:779:LEU:HD12	1:A:780:PRO:CD	2.49	0.43
1:A:501:LYS:HE2	1:A:501:LYS:HB3	1.88	0.42
1:A:738:VAL:HG22	1:A:779:LEU:HD13	2.02	0.42
1:A:989:PRO:HG2	1:A:1080:TRP:NE1	2.35	0.42
1:A:355:TRP:NE1	1:A:601:GLN:NE2	2.67	0.42
1:A:779:LEU:HD12	1:A:780:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:947:ARG:CD	1:A:968:ILE:HG21	2.48	0.42
1:A:158:ILE:HG23	1:A:703:ILE:HD13	2.01	0.42
1:A:164:ASP:OD2	1:A:165:VAL:N	2.52	0.42
1:A:214:LYS:HZ2	1:A:214:LYS:HB3	1.84	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HH11	1.84	0.42
1:A:486:GLN:O	1:A:487:ILE:HD13	2.19	0.42
1:A:235:VAL:HG21	1:A:244:ILE:HD13	2.01	0.42
1:A:622:LEU:HD12	1:A:623:ASP:N	2.35	0.42
1:A:306:VAL:HG22	1:A:306:VAL:O	2.20	0.42
1:A:865:LEU:HD11	1:A:959:ASN:ND2	2.34	0.42
1:A:155:THR:O	1:A:155:THR:HG22	2.19	0.42
1:A:632:ASP:OD1	1:A:634:ASN:HB2	2.20	0.42
1:A:199:HIS:O	1:A:200:PRO:C	2.57	0.42
1:A:896:VAL:CG1	1:A:901:ALA:HB3	2.50	0.42
1:A:997:THR:HG23	1:A:1001:LYS:HB3	2.01	0.42
1:A:893:GLN:HE21	1:A:893:GLN:HB3	1.61	0.42
1:A:287:ILE:HD12	1:A:288:LYS:H	1.84	0.42
1:A:379:LEU:HD13	1:A:379:LEU:HA	1.71	0.42
1:A:523:TYR:N	1:A:523:TYR:HD1	2.09	0.42
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.81	0.42
1:A:749:ILE:HG21	1:A:803:VAL:CG2	2.45	0.42
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.55	0.42
1:A:627:THR:HG21	1:A:648:LEU:HD21	2.02	0.41
1:A:954:ILE:HG12	1:A:955:THR:N	2.35	0.41
1:A:915:SER:HA	1:A:916:PRO:HD3	1.90	0.41
1:A:498:ASN:HB2	1:A:1036:MET:O	2.20	0.41
1:A:589:TYR:N	1:A:590:PRO:CD	2.84	0.41
1:A:702:GLU:OE1	1:A:839:ARG:NH1	2.53	0.41
1:A:778:GLN:HB2	1:A:779:LEU:H	1.68	0.41
1:A:562:ASP:OD1	1:A:1052:ARG:HD2	2.20	0.41
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.84	0.41
1:A:145:GLU:CD	1:A:145:GLU:C	2.79	0.41
1:A:883:LYS:HD3	1:A:883:LYS:HA	1.86	0.41
1:A:1026:LEU:O	1:A:1029:ILE:CG2	2.69	0.41
1:A:1050:TYR:C	1:A:1050:TYR:CD2	2.93	0.41
1:A:149:ALA:O	1:A:152:ARG:HB2	2.20	0.41
1:A:162:VAL:CG1	1:A:714:ALA:HB1	2.49	0.41
1:A:753:SER:CB	1:A:809:LYS:HE3	2.50	0.41
1:A:1035:LEU:HD12	1:A:1048:ILE:HA	2.02	0.41
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.86	0.41
1:A:215:ILE:O	1:A:216:ALA:C	2.58	0.41
1:A:516:ILE:HG13	1:A:517:SER:H	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:907:LEU:HD23	1:A:911:LEU:HG	2.03	0.41
1:A:887:THR:HG21	1:A:950:ASP:HA	2.03	0.41
1:A:171:ASP:OD2	1:A:472:ARG:NH1	2.51	0.41
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.02	0.41
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.21	0.41
1:A:880:GLU:O	2:A:9999:ML9:H21B	2.21	0.41
1:A:900:GLY:O	1:A:902:PHE:N	2.45	0.41
1:A:168:VAL:HG22	1:A:170:ASP:H	1.86	0.40
1:A:171:ASP:OD1	1:A:472:ARG:NH2	2.49	0.40
1:A:302:GLU:HG3	1:A:304:HIS:HE2	1.86	0.40
1:A:786:PRO:HD2	1:A:878:MET:CE	2.51	0.40
1:A:364:LYS:HB3	1:A:519:LEU:HB3	2.03	0.40
1:A:244:ILE:O	1:A:245:LEU:HD23	2.21	0.40
1:A:927:ARG:HE	1:A:959:ASN:ND2	2.17	0.40
1:A:879:ILE:HG22	1:A:880:GLU:O	2.21	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	829/966 (86%)	748 (90%)	57 (7%)	24 (3%)	7 9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	525	HIS
1	A	530	PRO
1	A	548	PRO
1	A	1045	LYS
1	A	164	ASP
1	A	216	ALA
1	A	231	GLN
1	A	307	LEU

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Mol	Chain	Res	Type
1	A	523	TYR
1	A	524	CYS
1	A	561	THR
1	A	783	PHE
1	A	901	ALA
1	A	999	GLY
1	A	775	GLN
1	A	798	ILE
1	A	230	SER
1	A	521	ASP
1	A	549	ASN
1	A	210	TYR
1	A	956	GLU
1	A	896	VAL
1	A	1079	GLY
1	A	897	GLY

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	762/864 (88%)	703 (92%)	59 (8%)	18	32

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	152	ARG
1	A	207	LEU
1	A	225	HIS
1	A	240	THR
1	A	278	ASP
1	A	281	LEU
1	A	291	GLN
1	A	317	GLU
1	A	320	LYS
1	A	358	ASP

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Mol	Chain	Res	Type
1	A	366	ARG
1	A	370	ILE
1	A	379	LEU
1	A	381	VAL
1	A	404	PHE
1	A	459	ARG
1	A	496	SER
1	A	498	ASN
1	A	501	LYS
1	A	516	ILE
1	A	523	TYR
1	A	524	CYS
1	A	544	ARG
1	A	549	ASN
1	A	587	LYS
1	A	601	GLN
1	A	602	GLU
1	A	613	ARG
1	A	646	GLN
1	A	662	GLN
1	A	682	LEU
1	A	717	LEU
1	A	740	GLU
1	A	766	GLN
1	A	767	LEU
1	A	808	LYS
1	A	811	LEU
1	A	816	LYS
1	A	823	LEU
1	A	843	LEU
1	A	845	LEU
1	A	847	ILE
1	A	853	SER
1	A	858	GLU
1	A	893	GLN
1	A	918	GLU
1	A	948	HIS
1	A	957	THR
1	A	960	LEU
1	A	968	ILE
1	A	982	ARG
1	A	1026	LEU

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Mol	Chain	Res	Type
1	A	1034	MET
1	A	1039	MET
1	A	1041	GLN
1	A	1046	GLU
1	A	1060	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	225	HIS
1	A	246	GLN
1	A	291	GLN
1	A	391	GLN
1	A	498	ASN
1	A	565	ASN
1	A	609	GLN
1	A	734	GLN
1	A	766	GLN
1	A	834	HIS
1	A	893	GLN
1	A	908	ASN
1	A	959	ASN
1	A	967	HIS
1	A	971	ASN
1	A	1060	ASN
1	A	1083	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ML9	A	9999	-	34,34,34	2.00	11 (32%)	46,48,48	1.42	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ML9	A	9999	-	-	0/14/24/24	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9999	ML9	C16-N17	4.93	1.39	1.32
2	A	9999	ML9	C8-C9	3.94	1.52	1.44
2	A	9999	ML9	C4-N7	3.66	1.45	1.39
2	A	9999	ML9	C6-N1	3.31	1.37	1.32
2	A	9999	ML9	C8-N7	3.12	1.43	1.38
2	A	9999	ML9	O19-C16	2.93	1.40	1.35
2	A	9999	ML9	C2-N12	2.57	1.39	1.34
2	A	9999	ML9	C10-C5	2.45	1.47	1.42
2	A	9999	ML9	C22-N7	2.24	1.52	1.49
2	A	9999	ML9	C18-C13	2.12	1.43	1.39
2	A	9999	ML9	C6-C5	-2.09	1.41	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9999	ML9	C2-N3-C4	3.52	119.52	115.30
2	A	9999	ML9	N3-C2-N1	-3.46	122.47	127.55
2	A	9999	ML9	C10-C5-C4	3.36	120.25	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9999	ML9	C9-C8-N7	2.76	118.02	116.13
2	A	9999	ML9	C5-C4-N7	-2.56	118.44	122.28
2	A	9999	ML9	C2-N1-C6	2.30	118.43	116.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	847/966 (87%)	0.55	52 (6%)	21 21	20, 58, 96, 118	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	SER	5.7
1	A	525	HIS	4.5
1	A	235	VAL	4.5
1	A	524	CYS	4.4
1	A	972	TYR	4.3
1	A	545	ALA	4.3
1	A	144	SER	4.0
1	A	270	PHE	3.8
1	A	898	ASN	3.7
1	A	771	LEU	3.6
1	A	774	LEU	3.6
1	A	1092	LEU	3.6
1	A	777	SER	3.4
1	A	249	PHE	3.4
1	A	216	ALA	3.3
1	A	1090	LEU	3.2
1	A	234	LYS	3.2
1	A	489	GLY	3.1
1	A	1082	VAL	3.0
1	A	779	LEU	3.0
1	A	146	GLU	2.9
1	A	778	GLN	2.9
1	A	352	VAL	2.9
1	A	215	ILE	2.8
1	A	404	PHE	2.8
1	A	244	ILE	2.7
1	A	271	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1041	GLN	2.6
1	A	902	PHE	2.5
1	A	1089	HIS	2.5
1	A	307	LEU	2.5
1	A	226	ARG	2.5
1	A	319	ARG	2.5
1	A	768	LYS	2.5
1	A	359	ARG	2.4
1	A	1084	PHE	2.4
1	A	901	ALA	2.3
1	A	741	MET	2.3
1	A	248	PHE	2.3
1	A	847	ILE	2.3
1	A	220	ILE	2.3
1	A	229	THR	2.2
1	A	823	LEU	2.2
1	A	320	LYS	2.2
1	A	151	GLN	2.1
1	A	869	CYS	2.1
1	A	544	ARG	2.1
1	A	660	LEU	2.1
1	A	929	VAL	2.1
1	A	231	GLN	2.1
1	A	435	CYS	2.0
1	A	907	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ML9	A	9999	31/31	0.20	0.03	42,48,68,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.