



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 03:05 PM EDT

PDB ID : 3ML8  
Title : Discovery of the Highly Potent PI3K/mTOR Dual Inhibitor PF-04691502 through Structure Based Drug Design  
Authors : Knighton, D.R.  
Deposited on : unknown  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

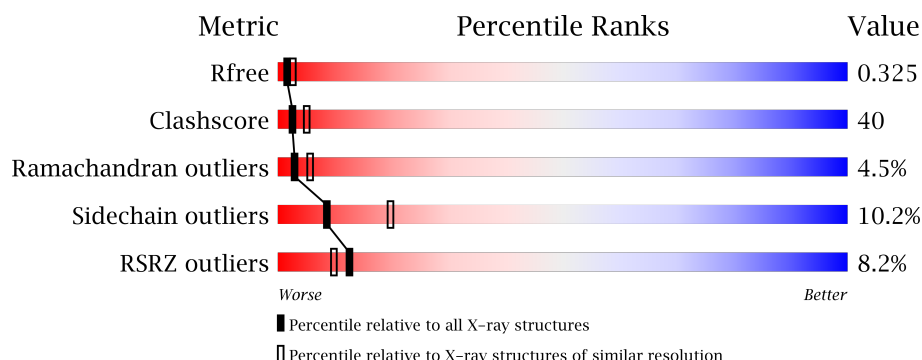
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	966	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6858 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.

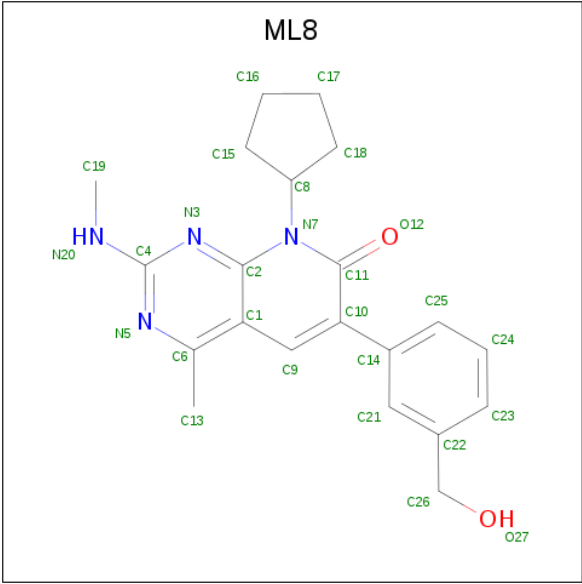
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	843	Total	C	N	O	S	0	0	0
			6831	4392	1162	1242	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	459	ARG	GLN	CONFLICT	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 8-cyclopentyl-6-[3-(hydroxymethyl)phenyl]-4-methyl-2-(methylamino)pyrido[2,3-d]pyrimidin-7(8H)-one (three-letter code: ML8) (formula: C<sub>21</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>).

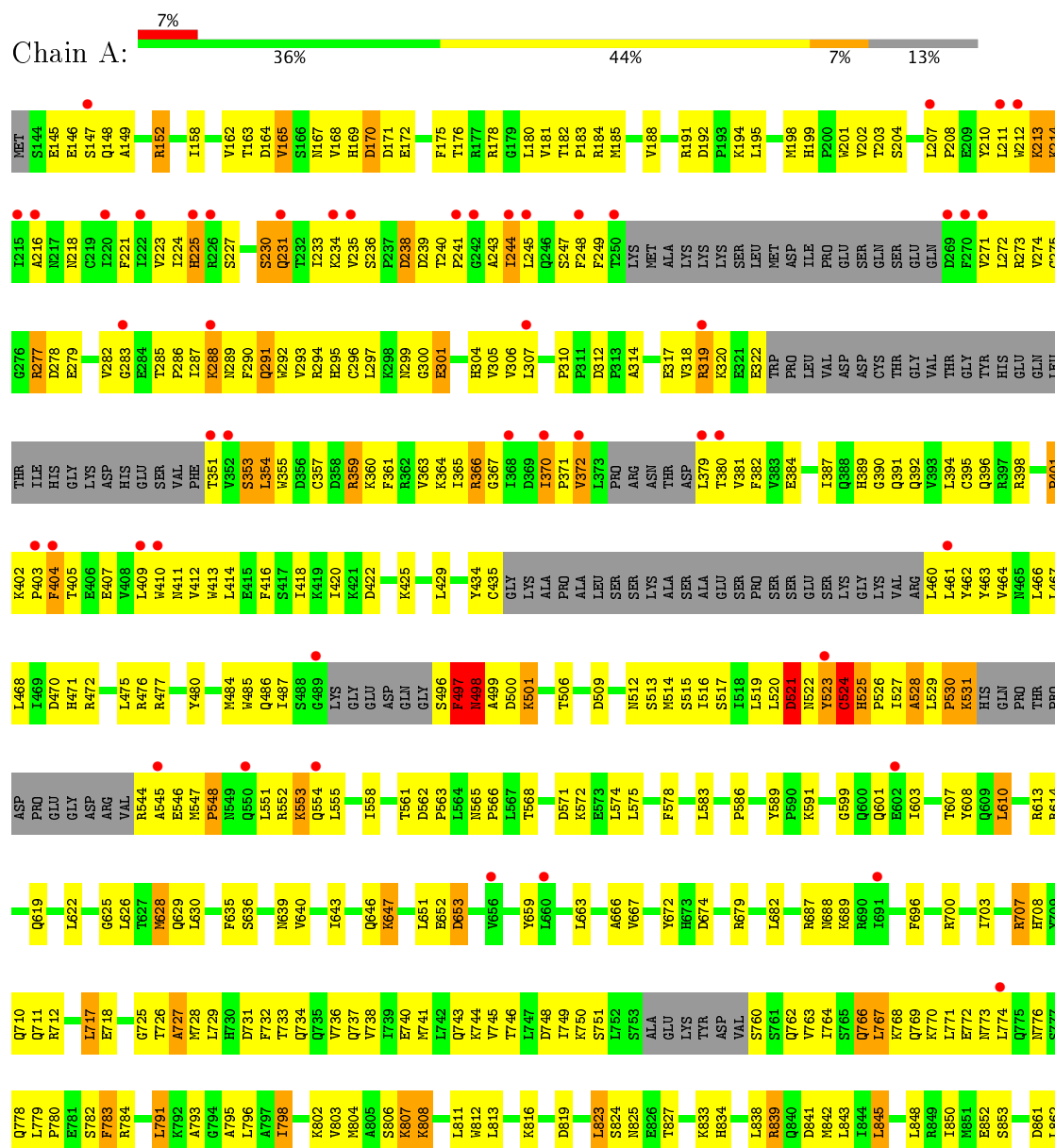


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	21	4	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.24Å 67.39Å 106.88Å 90.00° 95.12° 90.00°	Depositor
Resolution (Å)	37.54 – 2.70 44.72 – 2.52	Depositor EDS
% Data completeness (in resolution range)	95.2 (37.54-2.70) 94.6 (44.72-2.52)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.51Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.246 , 0.324 0.242 , 0.325	Depositor DCC
$R_{free}$ test set	1329 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ML8

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	0.41	0/6979	0.57	0/9443

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	497	PHE	Peptide
1	A	524	CYS	Peptide

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6831	0	6871	552	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	24	3	0
All	All	6858	0	6895	553	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 40.

All (553) 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:524:CYS:HB2	1:A:525:HIS:HA	1.28	1.09
1:A:524:CYS:CB	1:A:525:HIS:HA	1.87	1.04
1:A:351:THR:HG23	1:A:526:PRO:HB2	1.40	1.04
1:A:527:ILE:HA	1:A:528:ALA:HB2	1.36	1.02
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.26	0.98
1:A:568:THR:HG23	1:A:571:ASP:H	1.29	0.98
1:A:168:VAL:HG13	1:A:170:ASP:H	1.28	0.97
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.45	0.97
1:A:766:GLN:N	1:A:766:GLN:HE21	1.63	0.97
1:A:147:SER:HB3	1:A:319:ARG:HH21	1.28	0.95
1:A:527:ILE:HA	1:A:528:ALA:CB	1.95	0.95
1:A:466:LEU:HD11	1:A:476:ARG:HH11	1.28	0.94
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.50	0.94
1:A:387:ILE:HD12	1:A:418:ILE:HD12	1.49	0.93
1:A:149:ALA:HA	1:A:152:ARG:NH1	1.85	0.90
1:A:524:CYS:HB2	1:A:525:HIS:CA	2.03	0.88
1:A:766:GLN:H	1:A:766:GLN:HE21	0.91	0.87
1:A:149:ALA:HA	1:A:152:ARG:HH12	1.38	0.85
1:A:807:LYS:HE3	1:A:807:LYS:H	1.40	0.85
1:A:766:GLN:H	1:A:766:GLN:NE2	1.74	0.83
1:A:320:LYS:H	1:A:320:LYS:HD2	1.43	0.83
1:A:319:ARG:HG3	1:A:320:LYS:N	1.93	0.82
1:A:486:GLN:HG3	1:A:487:ILE:N	1.92	0.81
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	1.95	0.81
1:A:1044:SER:O	1:A:1045:LYS:HB3	1.79	0.81
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.64	0.80
1:A:273:ARG:O	1:A:305:VAL:HG13	1.83	0.79
1:A:1069:LEU:HD23	1:A:1072:ILE:HD12	1.63	0.79
1:A:767:LEU:O	1:A:771:LEU:HG	1.83	0.79
1:A:486:GLN:HG3	1:A:487:ILE:H	1.49	0.77
1:A:147:SER:HB3	1:A:319:ARG:NH2	2.00	0.77
1:A:527:ILE:CA	1:A:528:ALA:HB2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:ILE:O	1:A:768:LYS:HG2	1.86	0.76
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.67	0.76
1:A:467:LEU:HD13	1:A:672:TYR:CE2	2.21	0.76
1:A:568:THR:HG22	1:A:571:ASP:CG	2.06	0.76
1:A:689:LYS:HG2	1:A:728:MET:SD	2.26	0.75
1:A:477:ARG:NH1	1:A:525:HIS:ND1	2.35	0.75
1:A:921:PHE:O	1:A:925:VAL:HG23	1.87	0.75
1:A:750:LYS:NZ	1:A:834:HIS:HD2	1.85	0.74
1:A:380:THR:HA	1:A:402:LYS:O	1.86	0.74
1:A:360:LYS:HB3	1:A:416:PHE:O	1.88	0.74
1:A:803:VAL:HG12	1:A:804:MET:H	1.52	0.74
1:A:363:VAL:HG23	1:A:520:LEU:HD22	1.70	0.74
1:A:887:THR:HG21	1:A:950:ASP:HA	1.69	0.74
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.69	0.74
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.68	0.74
1:A:529:LEU:HD12	1:A:530:PRO:HD2	1.69	0.73
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.53	0.73
1:A:947:ARG:HD3	1:A:968:ILE:HD13	1.70	0.73
1:A:750:LYS:HZ3	1:A:834:HIS:HD2	1.35	0.72
1:A:162:VAL:HG21	1:A:718:GLU:OE1	1.89	0.72
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.72	0.71
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.55	0.71
1:A:351:THR:CG2	1:A:526:PRO:HB2	2.19	0.70
1:A:927:ARG:O	1:A:931:SER:HB3	1.90	0.70
1:A:1055:LEU:O	1:A:1056:THR:HG22	1.91	0.70
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.07	0.70
1:A:1026:LEU:O	1:A:1029:ILE:HG22	1.90	0.70
1:A:1056:THR:O	1:A:1056:THR:HG23	1.91	0.70
1:A:882:VAL:HG23	2:A:9999:ML8:H13	1.74	0.70
1:A:514:MET:HG3	1:A:515:SER:N	2.08	0.69
1:A:466:LEU:CD1	1:A:476:ARG:HH11	2.04	0.69
1:A:798:ILE:HD13	1:A:798:ILE:H	1.56	0.69
1:A:887:THR:CG2	1:A:950:ASP:HA	2.22	0.69
1:A:287:ILE:HG13	1:A:288:LYS:H	1.58	0.69
1:A:236:SER:HB3	1:A:239:ASP:OD1	1.93	0.68
1:A:152:ARG:HB2	1:A:152:ARG:HH11	1.58	0.68
1:A:748:ASP:HB3	1:A:770:LYS:NZ	2.09	0.68
1:A:354:LEU:HD23	1:A:355:TRP:CD1	2.28	0.68
1:A:795:ALA:HB3	1:A:816:LYS:HE2	1.74	0.68
1:A:896:VAL:HG12	1:A:899:THR:HB	1.76	0.68
1:A:905:GLU:O	1:A:905:GLU:HG2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:SER:O	1:A:497:PHE:HB2	1.93	0.68
1:A:524:CYS:CB	1:A:525:HIS:CA	2.68	0.68
1:A:1005:HIS:CE1	1:A:1008:LYS:HZ1	2.12	0.68
1:A:1045:LYS:HE3	1:A:1049:GLU:HG3	1.74	0.68
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.58	0.67
1:A:230:SER:O	1:A:231:GLN:HB2	1.95	0.67
1:A:198:MET:SD	1:A:282:VAL:HG21	2.34	0.67
1:A:748:ASP:HB3	1:A:770:LYS:HZ1	1.58	0.67
1:A:903:LYS:HE2	1:A:905:GLU:HB3	1.74	0.67
1:A:625:GLY:O	1:A:629:GLN:HG3	1.94	0.67
1:A:243:ALA:C	1:A:245:LEU:H	1.97	0.66
1:A:767:LEU:HD12	1:A:803:VAL:CG2	2.25	0.66
1:A:954:ILE:HG12	1:A:955:THR:N	2.10	0.66
1:A:614:ARG:HG2	1:A:614:ARG:O	1.95	0.66
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.60	0.66
1:A:807:LYS:HE3	1:A:807:LYS:N	2.10	0.66
1:A:1017:TYR:O	1:A:1021:ARG:HG3	1.95	0.66
1:A:498:ASN:HD22	1:A:499:ALA:N	1.93	0.66
1:A:803:VAL:HG12	1:A:804:MET:N	2.11	0.66
1:A:1045:LYS:HA	1:A:1048:ILE:HD12	1.76	0.66
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.60	0.66
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.31	0.66
1:A:525:HIS:O	1:A:527:ILE:HG13	1.95	0.66
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.07	0.66
1:A:204:SER:HB2	1:A:652:GLU:OE2	1.97	0.65
1:A:1010:GLN:O	1:A:1014:VAL:HG23	1.96	0.65
1:A:184:ARG:O	1:A:188:VAL:HG23	1.96	0.65
1:A:282:VAL:HG12	1:A:283:GLY:H	1.61	0.65
1:A:171:ASP:CG	1:A:472:ARG:HH22	1.99	0.65
1:A:477:ARG:HH21	1:A:521:ASP:HB3	1.61	0.65
1:A:271:VAL:HG21	1:A:282:VAL:HG22	1.79	0.64
1:A:524:CYS:HB2	1:A:525:HIS:CG	2.31	0.64
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.80	0.64
1:A:475:LEU:N	1:A:527:ILE:O	2.23	0.64
1:A:1024:THR:HG22	1:A:1028:ILE:CD1	2.26	0.64
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.79	0.64
1:A:379:LEU:O	1:A:404:PHE:HB2	1.97	0.64
1:A:990:ASP:O	1:A:994:VAL:HG23	1.98	0.64
1:A:165:VAL:O	1:A:165:VAL:HG12	1.96	0.64
1:A:930:TYR:CD2	1:A:1012:ILE:HD13	2.33	0.63
1:A:241:PRO:HD3	1:A:285:THR:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:TRP:HE3	1:A:911:LEU:HD23	1.64	0.63
1:A:198:MET:CE	1:A:282:VAL:HG11	2.29	0.63
1:A:1082:VAL:HA	1:A:1085:ASN:HB2	1.81	0.63
1:A:235:VAL:HG13	1:A:239:ASP:OD2	1.99	0.63
1:A:939:THR:OG1	1:A:945:GLY:HA2	1.97	0.63
1:A:1067:TYR:O	1:A:1071:GLN:HG2	1.97	0.63
1:A:1068:PHE:O	1:A:1071:GLN:HB2	1.98	0.63
1:A:470:ASP:CB	1:A:476:ARG:HH21	2.11	0.63
1:A:741:MET:O	1:A:745:VAL:HG23	1.99	0.62
1:A:463:TYR:CD2	1:A:487:ILE:HD11	2.34	0.62
1:A:947:ARG:HD3	1:A:968:ILE:HG21	1.81	0.62
1:A:778:GLN:H	1:A:778:GLN:CD	2.03	0.62
1:A:486:GLN:O	1:A:487:ILE:HD13	1.99	0.62
1:A:966:GLY:O	1:A:970:GLY:HA3	1.99	0.62
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.82	0.62
1:A:862:LEU:N	1:A:862:LEU:HD23	2.14	0.62
1:A:1068:PHE:O	1:A:1072:ILE:HG13	1.99	0.62
1:A:734:GLN:NE2	1:A:780:PRO:HB2	2.15	0.62
1:A:1042:LEU:HD23	1:A:1047:ASP:OD2	2.01	0.61
1:A:903:LYS:HD3	1:A:906:VAL:HG23	1.82	0.61
1:A:233:ILE:HG22	1:A:234:LYS:O	2.00	0.61
1:A:371:PRO:O	1:A:372:VAL:HB	2.01	0.61
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.34	0.61
1:A:1009:PHE:HA	1:A:1012:ILE:HD12	1.83	0.61
1:A:293:VAL:O	1:A:297:LEU:HG	2.01	0.61
1:A:812:TRP:O	1:A:812:TRP:CD1	2.53	0.61
1:A:935:TYR:O	1:A:939:THR:HG22	2.01	0.61
1:A:390:GLY:CA	1:A:636:SER:HB2	2.29	0.61
1:A:931:SER:OG	1:A:960:LEU:HB3	2.00	0.61
1:A:188:VAL:HG11	1:A:318:VAL:HG21	1.82	0.61
1:A:812:TRP:O	1:A:812:TRP:HD1	1.84	0.60
1:A:523:TYR:O	1:A:525:HIS:HB2	2.01	0.60
1:A:525:HIS:HB3	1:A:527:ILE:CD1	2.31	0.60
1:A:382:PHE:CE2	1:A:398:ARG:HD3	2.37	0.60
1:A:498:ASN:C	1:A:498:ASN:HD22	2.04	0.60
1:A:212:TRP:C	1:A:214:LYS:H	2.04	0.60
1:A:207:LEU:CB	1:A:288:LYS:HE3	2.31	0.60
1:A:410:TRP:HB3	1:A:412:VAL:HG13	1.82	0.60
1:A:477:ARG:HD3	1:A:522:ASN:HA	1.84	0.59
1:A:149:ALA:CA	1:A:152:ARG:HH12	2.14	0.59
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:ILE:O	1:A:906:VAL:HG11	2.03	0.59
1:A:1021:ARG:NE	1:A:1056:THR:HG22	2.17	0.59
1:A:1024:THR:HG22	1:A:1028:ILE:HD12	1.85	0.59
1:A:245:LEU:C	1:A:247:SER:H	2.04	0.59
1:A:568:THR:HG23	1:A:571:ASP:N	2.10	0.59
1:A:659:TYR:O	1:A:663:LEU:HG	2.01	0.59
1:A:320:LYS:HD2	1:A:320:LYS:N	2.16	0.58
1:A:903:LYS:HD3	1:A:906:VAL:CG2	2.33	0.58
1:A:925:VAL:O	1:A:929:VAL:HG23	2.04	0.58
1:A:883:LYS:O	1:A:884:ASP:HB2	2.04	0.58
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.39	0.57
1:A:935:TYR:O	1:A:939:THR:HB	2.03	0.57
1:A:1089:HIS:HA	1:A:1093:GLY:HA2	1.85	0.57
1:A:145:GLU:HG2	1:A:148:GLN:OE1	2.04	0.57
1:A:351:THR:HG23	1:A:526:PRO:CB	2.25	0.57
1:A:798:ILE:CD1	1:A:798:ILE:H	2.12	0.57
1:A:937:VAL:O	1:A:941:VAL:HG23	2.03	0.57
1:A:1045:LYS:CE	1:A:1049:GLU:HG3	2.35	0.57
1:A:282:VAL:HG12	1:A:283:GLY:N	2.19	0.57
1:A:463:TYR:HD2	1:A:487:ILE:HD11	1.69	0.57
1:A:524:CYS:HB2	1:A:525:HIS:CD2	2.40	0.57
1:A:760:SER:OG	1:A:763:VAL:HG23	2.05	0.57
1:A:168:VAL:HG13	1:A:170:ASP:N	2.09	0.57
1:A:176:THR:HG23	1:A:674:ASP:CB	2.29	0.57
1:A:230:SER:O	1:A:231:GLN:CB	2.53	0.57
1:A:811:LEU:HD23	1:A:813:LEU:HD21	1.87	0.57
1:A:782:SER:O	1:A:783:PHE:HB3	2.04	0.57
1:A:235:VAL:HG21	1:A:244:ILE:HD13	1.87	0.56
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.29	0.56
1:A:568:THR:HG22	1:A:571:ASP:OD2	2.05	0.56
1:A:750:LYS:HZ1	1:A:808:LYS:HB3	1.69	0.56
1:A:861:ASP:C	1:A:862:LEU:HD23	2.25	0.56
1:A:272:LEU:CD2	1:A:305:VAL:HG11	2.34	0.56
1:A:887:THR:HG21	1:A:950:ASP:OD1	2.05	0.56
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.87	0.56
1:A:983:VAL:HG23	1:A:984:PRO:HD2	1.88	0.56
1:A:524:CYS:HB3	1:A:526:PRO:HD2	1.88	0.56
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.35	0.56
1:A:750:LYS:NZ	1:A:834:HIS:CD2	2.71	0.56
1:A:562:ASP:OD1	1:A:1052:ARG:HD2	2.06	0.56
1:A:750:LYS:HZ3	1:A:834:HIS:CD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:TYR:O	1:A:939:THR:CG2	2.55	0.55
1:A:287:ILE:C	1:A:289:ASN:H	2.09	0.55
1:A:887:THR:HG22	1:A:889:ALA:N	2.21	0.55
1:A:240:THR:HG23	1:A:243:ALA:CB	2.37	0.55
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.22	0.55
1:A:885:ALA:HB2	1:A:955:THR:HG22	1.87	0.55
1:A:928:PHE:HZ	1:A:991:PHE:CD1	2.25	0.55
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.07	0.55
1:A:168:VAL:HG13	1:A:169:HIS:N	2.21	0.55
1:A:530:PRO:O	1:A:531:LYS:HB3	2.07	0.55
1:A:725:GLY:O	1:A:727:ALA:N	2.39	0.55
1:A:955:THR:C	1:A:957:THR:H	2.09	0.55
1:A:287:ILE:HG13	1:A:288:LYS:N	2.19	0.55
1:A:547:MET:HE1	1:A:552:ARG:HA	1.88	0.55
1:A:523:TYR:O	1:A:525:HIS:CB	2.54	0.54
1:A:687:ARG:HG2	1:A:687:ARG:O	2.06	0.54
1:A:774:LEU:O	1:A:779:LEU:HB3	2.07	0.54
1:A:916:PRO:HG3	1:A:920:LYS:HD3	1.87	0.54
1:A:198:MET:HE1	1:A:282:VAL:HG11	1.90	0.54
1:A:359:ARG:HH11	1:A:359:ARG:HB2	1.72	0.54
1:A:271:VAL:CG2	1:A:282:VAL:HG22	2.37	0.54
1:A:477:ARG:NH1	1:A:525:HIS:HD1	2.03	0.54
1:A:171:ASP:OD1	1:A:472:ARG:NH2	2.36	0.54
1:A:223:VAL:CG1	1:A:225:HIS:HE1	2.20	0.54
1:A:319:ARG:HG3	1:A:320:LYS:H	1.70	0.54
1:A:811:LEU:N	1:A:811:LEU:HD12	2.23	0.54
1:A:887:THR:HG22	1:A:889:ALA:H	1.72	0.54
1:A:366:ARG:HB2	1:A:517:SER:HB2	1.89	0.54
1:A:277:ARG:HH22	1:A:791:LEU:HG	1.72	0.54
1:A:995:MET:O	1:A:1005:HIS:HB2	2.07	0.54
1:A:202:VAL:HG12	1:A:203:THR:N	2.22	0.54
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.72	0.54
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.38	0.54
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.40	0.54
1:A:207:LEU:HB3	1:A:288:LYS:HE3	1.90	0.54
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.20	0.54
1:A:985:PHE:CD2	1:A:985:PHE:N	2.76	0.54
1:A:933:ALA:HB1	1:A:1013:CYS:SG	2.48	0.54
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.42	0.54
1:A:989:PRO:HG2	1:A:1080:TRP:NE1	2.23	0.54
1:A:476:ARG:HD3	1:A:480:TYR:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:LEU:HA	1:A:635:PHE:CD1	2.43	0.53
1:A:968:ILE:C	1:A:970:GLY:H	2.11	0.53
1:A:176:THR:CG2	1:A:674:ASP:HB2	2.31	0.53
1:A:930:TYR:HD2	1:A:1012:ILE:HD13	1.74	0.53
1:A:1002:THR:HG22	1:A:1002:THR:O	2.09	0.53
1:A:1069:LEU:O	1:A:1073:GLU:HG2	2.09	0.53
1:A:290:PHE:O	1:A:294:ARG:HG3	2.08	0.53
1:A:381:VAL:HB	1:A:404:PHE:CD2	2.43	0.53
1:A:299:ASN:HB2	1:A:301:GLU:OE1	2.09	0.53
1:A:524:CYS:HB3	1:A:525:HIS:HA	1.85	0.53
1:A:816:LYS:NZ	1:A:816:LYS:HB2	2.23	0.53
1:A:202:VAL:CG1	1:A:203:THR:N	2.71	0.53
1:A:165:VAL:O	1:A:165:VAL:CG1	2.57	0.53
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.42	0.53
1:A:783:PHE:CE1	1:A:793:ALA:HB3	2.44	0.53
1:A:960:LEU:HG	1:A:961:PHE:N	2.24	0.53
1:A:948:HIS:N	1:A:948:HIS:CD2	2.77	0.53
1:A:181:VAL:HG12	1:A:185:MET:CE	2.39	0.53
1:A:223:VAL:HG12	1:A:225:HIS:HE1	1.73	0.53
1:A:353:SER:HA	1:A:528:ALA:HB1	1.89	0.53
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.74	0.52
1:A:370:ILE:O	1:A:370:ILE:HG23	2.10	0.52
1:A:461:LEU:HB3	1:A:462:TYR:CE2	2.44	0.52
1:A:353:SER:HA	1:A:528:ALA:CB	2.40	0.52
1:A:910:TRP:CE3	1:A:911:LEU:HD23	2.45	0.52
1:A:917:THR:OG1	1:A:919:GLU:N	2.42	0.52
1:A:968:ILE:HG13	1:A:969:LEU:H	1.74	0.52
1:A:1043:THR:C	1:A:1045:LYS:H	2.13	0.52
1:A:240:THR:HG23	1:A:243:ALA:HB2	1.91	0.52
1:A:402:LYS:HG3	1:A:403:PRO:HD2	1.90	0.52
1:A:162:VAL:HG23	1:A:163:THR:N	2.24	0.52
1:A:935:TYR:O	1:A:939:THR:CB	2.57	0.52
1:A:990:ASP:OD2	1:A:990:ASP:N	2.43	0.52
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.36	0.52
1:A:770:LYS:O	1:A:773:ASN:HB2	2.10	0.52
1:A:1052:ARG:HG3	1:A:1057:VAL:HG11	1.91	0.52
1:A:207:LEU:HB2	1:A:288:LYS:HE3	1.92	0.52
1:A:732:PHE:O	1:A:736:VAL:HG23	2.09	0.52
1:A:767:LEU:CD2	1:A:771:LEU:HD11	2.40	0.52
1:A:152:ARG:NH1	1:A:152:ARG:HB2	2.25	0.51
1:A:640:VAL:O	1:A:643:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH2	1:A:791:LEU:HG	2.25	0.51
1:A:1024:THR:HG22	1:A:1028:ILE:HD11	1.93	0.51
1:A:1081:THR:O	1:A:1085:ASN:HB2	2.11	0.51
1:A:239:ASP:O	1:A:287:ILE:HG23	2.11	0.51
1:A:287:ILE:C	1:A:289:ASN:N	2.62	0.51
1:A:746:THR:HG23	1:A:811:LEU:HD13	1.93	0.51
1:A:907:LEU:O	1:A:911:LEU:HG	2.11	0.51
1:A:145:GLU:HA	1:A:148:GLN:HB2	1.93	0.51
1:A:243:ALA:C	1:A:245:LEU:N	2.64	0.51
1:A:372:VAL:HG13	1:A:372:VAL:O	2.10	0.51
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.92	0.51
1:A:274:VAL:HG23	1:A:279:GLU:O	2.11	0.51
1:A:746:THR:HA	1:A:811:LEU:HD11	1.93	0.51
1:A:886:THR:HG22	1:A:890:LYS:CD	2.41	0.51
1:A:1021:ARG:C	1:A:1023:HIS:H	2.14	0.50
1:A:287:ILE:O	1:A:289:ASN:N	2.44	0.50
1:A:861:ASP:C	1:A:861:ASP:OD1	2.48	0.50
1:A:434:TYR:CE1	1:A:460:LEU:HB2	2.46	0.50
1:A:915:SER:CB	1:A:921:PHE:HB2	2.41	0.50
1:A:182:THR:N	1:A:183:PRO:HD2	2.27	0.50
1:A:292:TRP:O	1:A:295:HIS:HB3	2.11	0.50
1:A:202:VAL:HG13	1:A:285:THR:HG21	1.93	0.50
1:A:707:ARG:HA	1:A:710:GLN:OE1	2.11	0.50
1:A:981:GLU:C	1:A:982:ARG:HG3	2.31	0.50
1:A:1045:LYS:HA	1:A:1048:ILE:CD1	2.42	0.50
1:A:198:MET:O	1:A:199:HIS:C	2.49	0.50
1:A:245:LEU:C	1:A:247:SER:N	2.65	0.50
1:A:274:VAL:HG12	1:A:275:CYS:N	2.26	0.50
1:A:212:TRP:C	1:A:214:LYS:N	2.65	0.50
1:A:395:CYS:SG	1:A:396:GLN:N	2.85	0.50
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.93	0.50
1:A:878:MET:C	1:A:879:ILE:HG13	2.32	0.50
1:A:244:ILE:O	1:A:244:ILE:HG22	2.12	0.50
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.42	0.49
1:A:743:GLN:HG2	1:A:876:ILE:HD11	1.94	0.49
1:A:918:GLU:O	1:A:921:PHE:HB3	2.12	0.49
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.42	0.49
1:A:936:CYS:SG	1:A:985:PHE:CD1	3.06	0.49
1:A:526:PRO:C	1:A:527:ILE:HG13	2.33	0.49
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.93	0.49
1:A:997:THR:HG21	1:A:1076:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:HA	1:A:213:LYS:CD	2.43	0.49
1:A:180:LEU:HD22	1:A:682:LEU:HD12	1.94	0.49
1:A:583:LEU:CD2	1:A:610:LEU:HD22	2.43	0.49
1:A:760:SER:O	1:A:764:ILE:HG13	2.13	0.49
1:A:839:ARG:HA	1:A:842:MET:HE2	1.94	0.49
1:A:841:ASP:O	1:A:845:LEU:HD22	2.11	0.49
1:A:370:ILE:HD13	1:A:371:PRO:N	2.28	0.49
1:A:667:VAL:O	1:A:712:ARG:NH1	2.46	0.49
1:A:773:ASN:O	1:A:776:ASN:HB2	2.13	0.49
1:A:364:LYS:HB2	1:A:413:TRP:CD2	2.48	0.48
1:A:434:TYR:CE1	1:A:460:LEU:HD13	2.48	0.48
1:A:462:TYR:HA	1:A:485:TRP:O	2.13	0.48
1:A:462:TYR:HB2	1:A:484:MET:HE2	1.94	0.48
1:A:286:PRO:O	1:A:289:ASN:HB2	2.12	0.48
1:A:364:LYS:HB2	1:A:413:TRP:CE2	2.48	0.48
1:A:401:PRO:O	1:A:402:LYS:HD3	2.12	0.48
1:A:425:LYS:HE2	1:A:672:TYR:CE1	2.47	0.48
1:A:955:THR:C	1:A:957:THR:N	2.65	0.48
1:A:1056:THR:CG2	1:A:1056:THR:O	2.61	0.48
1:A:509:ASP:CG	1:A:512:ASN:HD22	2.17	0.48
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.49	0.48
1:A:802:LYS:HG3	1:A:803:VAL:O	2.12	0.48
1:A:807:LYS:H	1:A:807:LYS:CE	2.18	0.48
1:A:477:ARG:CD	1:A:522:ASN:HA	2.43	0.48
1:A:390:GLY:HA2	1:A:636:SER:HB2	1.95	0.48
1:A:886:THR:HG22	1:A:890:LYS:HD3	1.95	0.48
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.78	0.48
1:A:180:LEU:C	1:A:183:PRO:HD2	2.34	0.48
1:A:806:SER:HB3	1:A:808:LYS:O	2.13	0.48
1:A:922:GLN:O	1:A:925:VAL:HB	2.13	0.48
1:A:501:LYS:HE2	1:A:501:LYS:HB3	1.58	0.48
1:A:529:LEU:HD12	1:A:530:PRO:CD	2.41	0.48
1:A:207:LEU:HD13	1:A:211:LEU:HB2	1.96	0.48
1:A:663:LEU:O	1:A:666:ALA:HB3	2.13	0.48
1:A:235:VAL:HG13	1:A:239:ASP:CB	2.44	0.48
1:A:273:ARG:CG	1:A:274:VAL:N	2.77	0.48
1:A:484:MET:SD	1:A:516:ILE:HB	2.54	0.48
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.95	0.48
1:A:1060:ASN:ND2	1:A:1060:ASN:H	2.12	0.47
1:A:862:LEU:HD11	1:A:1016:ALA:CB	2.42	0.47
1:A:953:MET:O	1:A:960:LEU:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:THR:O	1:A:407:GLU:N	2.47	0.47
1:A:167:ASN:ND2	1:A:506:THR:O	2.46	0.47
1:A:1008:LYS:O	1:A:1009:PHE:C	2.51	0.47
1:A:1007:GLN:HA	1:A:1010:GLN:OE1	2.15	0.47
1:A:552:ARG:HG2	1:A:553:LYS:HD3	1.96	0.47
1:A:823:LEU:HD12	1:A:823:LEU:H	1.80	0.47
1:A:496:SER:O	1:A:497:PHE:CB	2.61	0.47
1:A:525:HIS:HB3	1:A:527:ILE:HD12	1.96	0.47
1:A:811:LEU:N	1:A:811:LEU:CD1	2.78	0.47
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.49	0.47
1:A:381:VAL:HG13	1:A:381:VAL:O	2.15	0.47
1:A:1018:LEU:HD23	1:A:1021:ARG:HH11	1.80	0.46
1:A:475:LEU:HG	1:A:476:ARG:N	2.29	0.46
1:A:823:LEU:HD13	1:A:824:SER:N	2.29	0.46
1:A:355:TRP:CD1	1:A:601:GLN:NE2	2.83	0.46
1:A:887:THR:HB	1:A:890:LYS:HD2	1.97	0.46
1:A:198:MET:HE3	1:A:282:VAL:HG11	1.97	0.46
1:A:234:LYS:O	1:A:235:VAL:HG23	2.15	0.46
1:A:380:THR:OG1	1:A:401:PRO:HB3	2.15	0.46
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.74	0.46
1:A:568:THR:CG2	1:A:571:ASP:CG	2.82	0.46
1:A:607:THR:O	1:A:610:LEU:HB2	2.16	0.46
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.15	0.46
1:A:162:VAL:CG2	1:A:163:THR:N	2.79	0.46
1:A:364:LYS:HE3	1:A:411:ASN:O	2.15	0.46
1:A:555:LEU:HD13	1:A:574:LEU:CD1	2.46	0.46
1:A:949:ASN:HB2	1:A:1083:GLN:HE22	1.76	0.46
1:A:811:LEU:HB3	1:A:813:LEU:CD2	2.46	0.46
1:A:954:ILE:HG12	1:A:955:THR:H	1.80	0.46
1:A:225:HIS:HE2	1:A:304:HIS:HD2	1.64	0.46
1:A:466:LEU:CD1	1:A:476:ARG:NH1	2.77	0.46
1:A:547:MET:O	1:A:548:PRO:O	2.33	0.46
1:A:947:ARG:CD	1:A:968:ILE:HD13	2.45	0.46
1:A:509:ASP:O	1:A:513:SER:HB3	2.15	0.46
1:A:467:LEU:HD13	1:A:672:TYR:CD2	2.50	0.46
1:A:235:VAL:HG13	1:A:239:ASP:CG	2.36	0.45
1:A:434:TYR:CZ	1:A:460:LEU:HD13	2.50	0.45
1:A:462:TYR:CE2	1:A:514:MET:HE3	2.52	0.45
1:A:1043:THR:O	1:A:1045:LYS:N	2.49	0.45
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.32	0.45
1:A:852:GLU:HG2	1:A:864:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:TYR:CE1	1:A:639:ASN:ND2	2.85	0.45
1:A:990:ASP:OD2	1:A:1080:TRP:HZ2	1.99	0.45
1:A:1091:VAL:C	1:A:1092:LEU:HD23	2.37	0.45
1:A:145:GLU:C	1:A:147:SER:N	2.70	0.45
1:A:364:LYS:HG3	1:A:412:VAL:O	2.16	0.45
1:A:748:ASP:CB	1:A:770:LYS:NZ	2.78	0.45
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.51	0.45
1:A:464:VAL:CG1	1:A:484:MET:HG2	2.47	0.45
1:A:554:GLN:O	1:A:558:ILE:HG13	2.16	0.45
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.47	0.45
1:A:1058:GLY:HA3	1:A:1059:LYS:NZ	2.32	0.45
1:A:180:LEU:O	1:A:183:PRO:HD2	2.17	0.45
1:A:317:GLU:HG2	1:A:318:VAL:N	2.30	0.45
1:A:558:ILE:O	1:A:561:THR:HG22	2.16	0.45
1:A:168:VAL:CG1	1:A:169:HIS:N	2.78	0.45
1:A:273:ARG:HB3	1:A:306:VAL:HG13	1.98	0.45
1:A:294:ARG:HA	1:A:297:LEU:HD12	1.99	0.45
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.16	0.45
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.98	0.45
1:A:425:LYS:HB2	1:A:529:LEU:CD2	2.47	0.45
1:A:365:ILE:HG22	1:A:367:GLY:N	2.32	0.45
1:A:985:PHE:HB2	1:A:986:VAL:H	1.61	0.45
1:A:466:LEU:HD21	1:A:476:ARG:HD2	1.98	0.45
1:A:944:ILE:HB	1:A:968:ILE:HD12	1.98	0.45
1:A:379:LEU:O	1:A:404:PHE:N	2.50	0.44
1:A:717:LEU:HA	1:A:717:LEU:HD23	1.77	0.44
1:A:955:THR:O	1:A:957:THR:N	2.50	0.44
1:A:172:GLU:O	1:A:175:PHE:HB3	2.16	0.44
1:A:221:PHE:HD2	1:A:233:ILE:O	1.99	0.44
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.16	0.44
1:A:1083:GLN:HA	1:A:1083:GLN:NE2	2.32	0.44
1:A:207:LEU:HD22	1:A:208:PRO:HD2	1.99	0.44
1:A:214:LYS:HB3	1:A:214:LYS:HE2	1.82	0.44
1:A:249:PHE:N	1:A:249:PHE:CD2	2.82	0.44
1:A:850:ILE:HD13	1:A:1030:LEU:HD13	1.99	0.44
1:A:933:ALA:CB	1:A:1013:CYS:SG	3.05	0.44
1:A:146:GLU:OE2	1:A:146:GLU:HA	2.17	0.44
1:A:351:THR:HG23	1:A:526:PRO:C	2.38	0.44
1:A:750:LYS:NZ	1:A:834:HIS:O	2.50	0.44
1:A:207:LEU:CD1	1:A:211:LEU:HB2	2.48	0.44
1:A:370:ILE:HD13	1:A:370:ILE:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:CYS:H	1:A:418:ILE:HD11	1.83	0.44
1:A:1060:ASN:HD21	1:A:1063:ASP:CG	2.21	0.44
1:A:371:PRO:O	1:A:372:VAL:CB	2.64	0.44
1:A:466:LEU:HD11	1:A:476:ARG:NH1	2.12	0.44
1:A:874:ASP:O	1:A:875:LYS:HB2	2.17	0.44
1:A:865:LEU:HD12	1:A:961:PHE:CD2	2.53	0.44
1:A:1008:LYS:HG2	1:A:1012:ILE:HD11	2.00	0.44
1:A:145:GLU:C	1:A:147:SER:H	2.19	0.43
1:A:225:HIS:N	1:A:305:VAL:O	2.49	0.43
1:A:674:ASP:CG	1:A:679:ARG:HE	2.21	0.43
1:A:736:VAL:O	1:A:740:GLU:HB2	2.18	0.43
1:A:887:THR:HB	1:A:890:LYS:HG3	1.99	0.43
1:A:192:ASP:C	1:A:192:ASP:OD1	2.56	0.43
1:A:380:THR:O	1:A:435:CYS:HB2	2.18	0.43
1:A:367:GLY:HA3	1:A:409:LEU:HA	2.01	0.43
1:A:772:GLU:O	1:A:773:ASN:C	2.55	0.43
1:A:936:CYS:O	1:A:939:THR:HG22	2.19	0.43
1:A:210:TYR:HA	1:A:213:LYS:HD3	1.98	0.43
1:A:322:GLU:CD	1:A:322:GLU:H	2.21	0.43
1:A:548:PRO:HD2	1:A:551:LEU:HD12	2.00	0.43
1:A:947:ARG:NH2	1:A:951:ASN:HB3	2.34	0.43
1:A:1000:LYS:HB3	1:A:1000:LYS:HE3	1.77	0.43
1:A:1006:PHE:CE2	1:A:1010:GLN:CD	2.92	0.43
1:A:178:ARG:NH1	1:A:178:ARG:HG3	2.28	0.43
1:A:525:HIS:HB3	1:A:527:ILE:HD11	1.99	0.43
1:A:527:ILE:CA	1:A:528:ALA:CB	2.74	0.43
1:A:561:THR:HG23	1:A:591:LYS:NZ	2.34	0.43
1:A:745:VAL:O	1:A:749:ILE:HD12	2.18	0.43
1:A:968:ILE:O	1:A:970:GLY:N	2.51	0.43
1:A:422:ASP:HB3	1:A:599:GLY:O	2.19	0.43
1:A:496:SER:HB2	1:A:1044:SER:HA	2.01	0.43
1:A:381:VAL:HA	1:A:434:TYR:O	2.19	0.43
1:A:989:PRO:HD3	1:A:1079:GLY:O	2.19	0.43
1:A:207:LEU:HB2	1:A:288:LYS:CE	2.49	0.43
1:A:547:MET:HA	1:A:548:PRO:HD3	1.85	0.43
1:A:628:MET:HE2	1:A:628:MET:HB3	1.77	0.43
1:A:824:SER:OG	1:A:825:ASN:N	2.48	0.43
1:A:622:LEU:HD21	1:A:651:LEU:HD21	2.00	0.42
1:A:891:ILE:HD13	1:A:910:TRP:CD2	2.53	0.42
1:A:912:LYS:HG3	1:A:921:PHE:CE1	2.54	0.42
1:A:798:ILE:HD13	1:A:798:ILE:N	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD12	1:A:372:VAL:O	2.19	0.42
1:A:398:ARG:O	1:A:414:LEU:HD21	2.18	0.42
1:A:939:THR:CG2	1:A:940:PHE:N	2.82	0.42
1:A:210:TYR:CD1	1:A:211:LEU:HG	2.55	0.42
1:A:674:ASP:OD1	1:A:679:ARG:NE	2.46	0.42
1:A:731:ASP:OD1	1:A:784:ARG:NE	2.47	0.42
1:A:734:GLN:O	1:A:738:VAL:HG23	2.19	0.42
1:A:907:LEU:HD22	1:A:994:VAL:HG21	2.01	0.42
1:A:967:HIS:O	1:A:970:GLY:N	2.48	0.42
1:A:547:MET:HE3	1:A:578:PHE:CD1	2.54	0.42
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.55	0.42
1:A:1023:HIS:O	1:A:1024:THR:C	2.56	0.42
1:A:1059:LYS:HA	1:A:1059:LYS:HD3	1.78	0.42
1:A:296:CYS:O	1:A:300:GLY:N	2.53	0.42
1:A:307:LEU:C	1:A:307:LEU:HD23	2.40	0.42
1:A:548:PRO:HG2	1:A:551:LEU:CD1	2.43	0.42
1:A:610:LEU:HA	1:A:610:LEU:HD23	1.80	0.42
1:A:749:ILE:HG21	1:A:803:VAL:CG2	2.50	0.42
1:A:918:GLU:OE2	1:A:922:GLN:NE2	2.53	0.42
1:A:954:ILE:CG1	1:A:955:THR:N	2.79	0.42
1:A:568:THR:O	1:A:572:LYS:HG3	2.20	0.42
1:A:603:ILE:HA	1:A:603:ILE:HD13	1.83	0.42
1:A:647:LYS:HA	1:A:647:LYS:HD2	1.90	0.42
1:A:879:ILE:HG22	1:A:880:GLU:O	2.20	0.42
1:A:889:ALA:O	1:A:892:GLN:HB2	2.20	0.42
1:A:171:ASP:O	1:A:171:ASP:CG	2.59	0.41
1:A:199:HIS:O	1:A:199:HIS:CD2	2.72	0.41
1:A:880:GLU:O	2:A:9999:ML8:H13B	2.20	0.41
1:A:158:ILE:HG23	1:A:703:ILE:HD13	2.01	0.41
1:A:384:GLU:HG3	1:A:398:ARG:HG2	2.02	0.41
1:A:850:ILE:HD13	1:A:1030:LEU:CD1	2.50	0.41
1:A:969:LEU:HD23	1:A:969:LEU:HA	1.84	0.41
1:A:224:ILE:C	1:A:225:HIS:ND1	2.74	0.41
1:A:477:ARG:CZ	1:A:522:ASN:O	2.69	0.41
1:A:188:VAL:HG13	1:A:191:ARG:CZ	2.51	0.41
1:A:236:SER:O	1:A:238:ASP:N	2.54	0.41
1:A:274:VAL:CG1	1:A:275:CYS:N	2.83	0.41
1:A:225:HIS:NE2	1:A:304:HIS:HD2	2.18	0.41
1:A:819:ASP:C	1:A:819:ASP:OD1	2.59	0.41
1:A:990:ASP:OD2	1:A:1080:TRP:CZ2	2.73	0.41
1:A:1021:ARG:C	1:A:1023:HIS:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ARG:NH1	1:A:525:HIS:CG	2.88	0.41
1:A:614:ARG:CZ	1:A:643:ILE:HG22	2.50	0.41
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.86	0.41
1:A:939:THR:HG23	1:A:940:PHE:N	2.35	0.41
1:A:364:LYS:NZ	1:A:411:ASN:ND2	2.69	0.41
2:A:9999:ML8:H25	2:A:9999:ML8:O12	2.21	0.41
1:A:243:ALA:O	1:A:245:LEU:N	2.54	0.41
1:A:273:ARG:HG3	1:A:274:VAL:H	1.86	0.41
1:A:1040:PRO:O	1:A:1041:GLN:HB2	2.20	0.41
1:A:271:VAL:HG12	1:A:310:PRO:HG3	2.03	0.41
1:A:816:LYS:HB2	1:A:816:LYS:HZ3	1.86	0.41
1:A:967:HIS:O	1:A:968:ILE:C	2.59	0.41
1:A:968:ILE:C	1:A:970:GLY:N	2.73	0.41
1:A:930:TYR:O	1:A:931:SER:C	2.59	0.41
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.30	0.40
1:A:802:LYS:HG2	1:A:812:TRP:HB3	2.03	0.40
1:A:986:VAL:O	1:A:986:VAL:HG12	2.20	0.40
1:A:1084:PHE:CZ	1:A:1088:LEU:HD11	2.57	0.40
1:A:470:ASP:HB2	1:A:476:ARG:HH21	1.86	0.40
1:A:523:TYR:O	1:A:525:HIS:CG	2.74	0.40
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.89	0.40
1:A:530:PRO:O	1:A:531:LYS:CB	2.68	0.40
1:A:696:PHE:CE2	1:A:700:ARG:HD2	2.57	0.40
1:A:389:HIS:O	1:A:392:GLN:HB2	2.21	0.40
1:A:548:PRO:CD	1:A:551:LEU:HD12	2.51	0.40
1:A:864:LEU:HD22	1:A:935:TYR:CE1	2.56	0.40
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.90	0.40
1:A:355:TRP:NE1	1:A:601:GLN:NE2	2.63	0.40
1:A:470:ASP:HB2	1:A:476:ARG:NH2	2.37	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	825/966 (85%)	684 (83%)	104 (13%)	37 (4%)	<b>3</b> <b>6</b>

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	A	227	SER
1	A	230	SER
1	A	231	GLN
1	A	288	LYS
1	A	372	VAL
1	A	497	PHE
1	A	498	ASN
1	A	523	TYR
1	A	528	ALA
1	A	530	PRO
1	A	548	PRO
1	A	726	THR
1	A	796	LEU
1	A	898	ASN
1	A	967	HIS
1	A	968	ILE
1	A	165	VAL
1	A	216	ALA
1	A	244	ILE
1	A	401	PRO
1	A	521	ASP
1	A	524	CYS
1	A	969	LEU
1	A	218	ASN
1	A	545	ALA
1	A	783	PHE
1	A	827	THR
1	A	1022	HIS
1	A	1080	TRP
1	A	213	LYS
1	A	394	LEU
1	A	727	ALA
1	A	897	GLY
1	A	904	ASP
1	A	1079	GLY
1	A	984	PRO

### 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	758/864 (88%)	681 (90%)	77 (10%)	8 20

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	170	ASP
1	A	194	LYS
1	A	214	LYS
1	A	225	HIS
1	A	238	ASP
1	A	277	ARG
1	A	278	ASP
1	A	291	GLN
1	A	301	GLU
1	A	319	ARG
1	A	353	SER
1	A	354	LEU
1	A	357	CYS
1	A	359	ARG
1	A	366	ARG
1	A	370	ILE
1	A	391	GLN
1	A	404	PHE
1	A	498	ASN
1	A	501	LYS
1	A	521	ASP
1	A	525	HIS
1	A	531	LYS
1	A	544	ARG
1	A	546	GLU
1	A	553	LYS
1	A	575	LEU
1	A	610	LEU
1	A	613	ARG

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Mol	Chain	Res	Type
1	A	619	GLN
1	A	626	LEU
1	A	628	MET
1	A	646	GLN
1	A	647	LYS
1	A	653	ASP
1	A	707	ARG
1	A	711	GLN
1	A	717	LEU
1	A	729	LEU
1	A	744	LYS
1	A	751	SER
1	A	762	GLN
1	A	766	GLN
1	A	767	LEU
1	A	769	GLN
1	A	791	LEU
1	A	798	ILE
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	839	ARG
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	853	SER
1	A	878	MET
1	A	886	THR
1	A	893	GLN
1	A	898	ASN
1	A	909	HIS
1	A	919	GLU
1	A	931	SER
1	A	948	HIS
1	A	972	TYR
1	A	985	PHE
1	A	990	ASP
1	A	1000	LYS
1	A	1026	LEU
1	A	1052	ARG

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Mol	Chain	Res	Type
1	A	1056	THR
1	A	1063	ASP
1	A	1085	ASN
1	A	1090	LEU
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	217	ASN
1	A	291	GLN
1	A	304	HIS
1	A	391	GLN
1	A	411	ASN
1	A	498	ASN
1	A	512	ASN
1	A	639	ASN
1	A	734	GLN
1	A	737	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	834	HIS
1	A	840	GLN
1	A	908	ASN
1	A	967	HIS
1	A	1007	GLN
1	A	1023	HIS
1	A	1025	ASN
1	A	1083	GLN
1	A	1089	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ML8	A	9999	-	27,30,30	2.75	8 (29%)	31,43,43	1.81	6 (19%)

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	ML8	A	9999	-	-	0/8/19/19	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9999	ML8	C25-C14	2.14	1.43	1.39
2	A	9999	ML8	C9-C1	2.26	1.46	1.42
2	A	9999	ML8	C21-C14	2.76	1.44	1.39
2	A	9999	ML8	C10-C14	2.85	1.54	1.49
2	A	9999	ML8	C11-N7	3.80	1.43	1.38
2	A	9999	ML8	C11-C10	5.06	1.55	1.44
2	A	9999	ML8	C6-N5	5.40	1.37	1.32
2	A	9999	ML8	C4-N20	9.45	1.42	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9999	ML8	C19-N20-C4	-4.77	117.83	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9999	ML8	N3-C4-N5	-3.04	121.64	126.23
2	A	9999	ML8	C9-C1-C2	2.64	120.14	117.01
2	A	9999	ML8	C10-C11-N7	2.72	118.00	116.11
2	A	9999	ML8	N20-C4-N3	4.19	121.02	116.95
2	A	9999	ML8	C4-N3-C2	4.22	119.93	115.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9999	ML8	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	843/966 (87%)	0.52	69 (8%) 12 10	29, 70, 105, 121	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	971	ASN	7.0
1	A	409	LEU	6.0
1	A	1090	LEU	5.2
1	A	244	ILE	5.0
1	A	216	ALA	4.9
1	A	995	MET	4.8
1	A	404	PHE	4.6
1	A	235	VAL	4.4
1	A	307	LEU	4.3
1	A	1082	VAL	4.1
1	A	379	LEU	3.9
1	A	250	THR	3.8
1	A	523	TYR	3.8
1	A	242	GLY	3.8
1	A	987	LEU	3.7
1	A	222	ILE	3.6
1	A	489	GLY	3.4
1	A	403	PRO	3.3
1	A	967	HIS	3.3
1	A	241	PRO	3.3
1	A	234	LYS	3.3
1	A	211	LEU	3.2
1	A	226	ARG	3.2
1	A	352	VAL	3.2
1	A	1092	LEU	3.2
1	A	1041	GLN	3.2
1	A	212	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1091	VAL	3.0
1	A	968	ILE	3.0
1	A	902	PHE	3.0
1	A	550	GLN	3.0
1	A	972	TYR	3.0
1	A	892	GLN	2.9
1	A	691	ILE	2.9
1	A	368	ILE	2.8
1	A	215	ILE	2.8
1	A	901	ALA	2.8
1	A	245	LEU	2.8
1	A	351	THR	2.7
1	A	231	GLN	2.7
1	A	283	GLY	2.7
1	A	207	LEU	2.7
1	A	220	ILE	2.7
1	A	147	SER	2.7
1	A	410	TRP	2.6
1	A	380	THR	2.6
1	A	461	LEU	2.6
1	A	248	PHE	2.5
1	A	271	VAL	2.5
1	A	1042	LEU	2.5
1	A	1087	PHE	2.4
1	A	545	ALA	2.4
1	A	319	ARG	2.4
1	A	269	ASP	2.4
1	A	991	PHE	2.3
1	A	288	LYS	2.3
1	A	372	VAL	2.3
1	A	981	GLU	2.2
1	A	370	ILE	2.2
1	A	225	HIS	2.2
1	A	602	GLU	2.2
1	A	970	GLY	2.2
1	A	554	GLN	2.1
1	A	270	PHE	2.1
1	A	660	LEU	2.1
1	A	656	VAL	2.1
1	A	868	GLY	2.0
1	A	1083	GLN	2.0
1	A	774	LEU	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ML8	A	9999	27/27	0.94	0.26	1.20	47,51,58,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.