



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:05 PM GMT

PDB ID : 1NQF  
Title : OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI, METHIONINE SUBSTITUTION CONSTRUCT FOR SE-MET SAD PHASING  
Authors : Chimento, D.P.; Mohanty, A.K.; Kadner, R.J.; Wiener, M.C.  
Deposited on : 2003-01-21  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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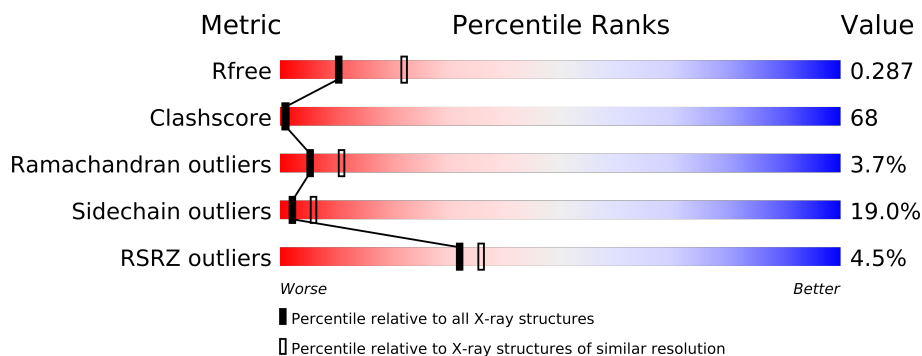
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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. 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	594	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	C8E	A	801	-	X
3	C8E	A	802	-	X
3	C8E	A	803	-	X
3	C8E	A	804	-	X
3	C8E	A	805	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4490 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 Vitamin B12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	Se	0	0	0
			4294	2700	740	846	8			

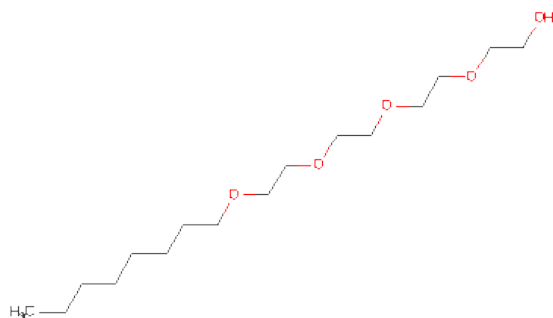
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	MSE	MET	ENGINEERED	UNP P06129
A	317	MSE	TRP	ENGINEERED	UNP P06129
A	319	MSE	LYS	ENGINEERED	UNP P06129
A	321	MSE	THR	ENGINEERED	UNP P06129
A	516	MSE	TRP	ENGINEERED	UNP P06129
A	518	MSE	ILE	ENGINEERED	UNP P06129
A	520	MSE	TYR	ENGINEERED	UNP P06129
A	541	MSE	MET	ENGINEERED	UNP P06129

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.61Å 81.61Å 226.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.70) 96.4 (29.99-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.244 , 0.288 0.244 , 0.287	Depositor DCC
$R_{free}$ test set	1222 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.6	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23965 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: MG, C8E

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	0.80	0/4384	1.04	20/5940 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASP	CB-CG-OD2	8.79	126.21	118.30
1	A	69	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	A	121	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	530	ASP	CB-CG-OD2	7.04	124.63	118.30
1	A	361	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	492	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	81	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	95	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	82	GLY	N-CA-C	6.05	128.24	113.10
1	A	274	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	241	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	45	VAL	CB-CA-C	-5.96	100.08	111.40
1	A	513	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	162	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	134	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	331	ASP	CB-CG-OD2	5.45	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	439	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	570	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	411	ASP	CB-CG-OD2	5.09	122.89	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	Peptide

## 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	4294	0	4071	560	1
2	A	1	0	0	0	0
3	A	126	0	204	67	0
4	A	69	0	0	16	0
All	All	4490	0	4275	589	1

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 68.

All (589) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:242:THR:HG21	1:A:277:TYR:CZ	1.52	1.45
1:A:89:GLY:HA3	1:A:91:SER:N	1.15	1.43
3:A:802:C8E:H52	3:A:802:C8E:C1	1.49	1.38
1:A:62:GLN:HE21	1:A:62:GLN:N	1.24	1.36
1:A:226:ARG:NH1	1:A:244:LYS:HG3	1.43	1.33
1:A:85:LEU:O	1:A:85:LEU:HD22	1.18	1.33
1:A:86:ASN:O	1:A:87:LEU:HD12	1.31	1.28
1:A:555:VAL:O	1:A:556:THR:HG23	1.18	1.27
1:A:18:PRO:O	1:A:21:THR:CG2	1.85	1.23

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:802:C8E:C5	3:A:802:C8E:H12	1.70	1.21
1:A:242:THR:CG2	1:A:277:TYR:CZ	2.23	1.19
1:A:198:LEU:C	1:A:198:LEU:HD12	1.59	1.18
1:A:85:LEU:O	1:A:85:LEU:CD2	1.92	1.17
1:A:559:LEU:O	1:A:559:LEU:HD22	1.43	1.17
1:A:89:GLY:HA3	1:A:90:VAL:C	1.58	1.17
1:A:91:SER:HB3	4:A:869:HOH:O	1.39	1.16
1:A:86:ASN:C	1:A:87:LEU:HD12	1.66	1.16
1:A:62:GLN:CA	1:A:62:GLN:HE21	1.54	1.16
1:A:245:LEU:HD23	1:A:246:TYR:N	1.59	1.15
1:A:120:SER:HB2	1:A:393:TYR:CE1	1.82	1.15
1:A:89:GLY:CA	1:A:91:SER:N	2.08	1.14
1:A:9:VAL:CG1	1:A:19:ARG:HD3	1.78	1.12
1:A:174:HIS:CE1	1:A:176:HIS:NE2	2.16	1.12
1:A:342:LEU:HD11	3:A:803:C8E:H51	1.17	1.12
1:A:9:VAL:HG11	1:A:19:ARG:HD3	1.15	1.11
1:A:245:LEU:CD2	1:A:246:TYR:N	2.15	1.10
1:A:160:LEU:HD22	1:A:166:VAL:HG21	1.20	1.09
1:A:62:GLN:NE2	1:A:62:GLN:N	1.98	1.09
1:A:61:GLY:C	1:A:62:GLN:HE21	1.55	1.09
1:A:169:LEU:C	1:A:169:LEU:HD12	1.75	1.07
1:A:555:VAL:C	1:A:556:THR:HG23	1.72	1.06
1:A:263:SER:HB2	1:A:302:ASN:HD22	1.18	1.06
1:A:103:LEU:HD23	1:A:103:LEU:N	1.71	1.05
1:A:120:SER:O	1:A:121:ASP:HB2	1.27	1.05
1:A:242:THR:HG21	1:A:277:TYR:OH	1.53	1.05
1:A:18:PRO:O	1:A:21:THR:HG22	0.88	1.04
1:A:88:ALA:O	1:A:92:GLY:HA2	1.56	1.04
1:A:226:ARG:HH22	1:A:244:LYS:HE2	1.21	1.03
3:A:803:C8E:H112	3:A:803:C8E:C16	1.88	1.03
1:A:198:LEU:HD12	1:A:199:SER:N	1.73	1.03
1:A:79:LEU:HB3	1:A:82:GLY:HA3	1.40	1.02
1:A:555:VAL:O	1:A:556:THR:CG2	2.06	1.02
1:A:226:ARG:HH12	1:A:244:LYS:CG	1.73	1.01
1:A:406:GLY:CA	1:A:452:LYS:HE3	1.89	1.01
1:A:226:ARG:HH12	1:A:244:LYS:HG3	0.95	1.01
1:A:160:LEU:CD2	1:A:166:VAL:HG21	1.91	1.01
1:A:263:SER:HB2	1:A:302:ASN:ND2	1.74	1.01
1:A:169:LEU:HD12	1:A:169:LEU:O	1.61	1.00
1:A:160:LEU:HD22	1:A:166:VAL:CG2	1.90	1.00
1:A:61:GLY:C	1:A:62:GLN:NE2	2.14	0.99
1:A:568:LEU:HB3	1:A:569:PHE:CD1	1.97	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:THR:O	1:A:326:THR:HB	1.63	0.99
1:A:362:ASN:HD22	1:A:365:PHE:H	1.12	0.98
1:A:160:LEU:CD2	1:A:166:VAL:CG2	2.42	0.98
1:A:120:SER:CB	1:A:393:TYR:CE1	2.47	0.97
1:A:398:LEU:H	1:A:398:LEU:CD2	1.77	0.97
1:A:496:LEU:O	1:A:497:ARG:HB2	1.60	0.97
1:A:147:ASN:O	1:A:148:SER:OG	1.81	0.96
1:A:198:LEU:CD1	1:A:198:LEU:C	2.27	0.96
1:A:174:HIS:CD2	1:A:174:HIS:C	2.38	0.96
1:A:539:VAL:HG23	1:A:540:LYS:N	1.77	0.96
1:A:18:PRO:HD2	1:A:21:THR:HG21	1.48	0.95
1:A:362:ASN:ND2	1:A:365:PHE:CD2	2.34	0.95
1:A:555:VAL:C	1:A:556:THR:CG2	2.34	0.94
1:A:342:LEU:CD1	3:A:803:C8E:H51	1.98	0.94
1:A:568:LEU:HB3	1:A:569:PHE:HD1	1.32	0.94
1:A:572:ASP:HA	4:A:864:HOH:O	1.67	0.94
1:A:406:GLY:HA3	1:A:452:LYS:CE	1.97	0.94
1:A:539:VAL:CG2	1:A:540:LYS:N	2.31	0.93
1:A:120:SER:O	1:A:121:ASP:CB	2.14	0.93
1:A:103:LEU:N	1:A:103:LEU:CD2	2.30	0.93
1:A:539:VAL:HG23	1:A:540:LYS:H	1.33	0.93
1:A:198:LEU:CD1	1:A:199:SER:N	2.32	0.92
1:A:245:LEU:HD23	1:A:246:TYR:H	1.27	0.92
1:A:555:VAL:HG12	1:A:556:THR:HG22	1.53	0.91
1:A:85:LEU:O	1:A:87:LEU:N	2.04	0.91
1:A:64:SER:O	1:A:95:ASP:OD1	1.89	0.91
1:A:464:VAL:HG11	3:A:804:C8E:H51	1.53	0.91
1:A:62:GLN:CA	1:A:62:GLN:NE2	2.25	0.90
1:A:559:LEU:C	1:A:559:LEU:HD22	1.90	0.90
1:A:518:MSE:HG3	1:A:549:LEU:CD1	2.02	0.89
1:A:323:THR:O	1:A:326:THR:CB	2.19	0.89
3:A:803:C8E:O15	3:A:803:C8E:H112	1.67	0.89
1:A:89:GLY:HA3	1:A:91:SER:H	1.37	0.89
1:A:224:ASP:OD1	1:A:224:ASP:O	1.89	0.89
1:A:506:GLN:NE2	1:A:519:THR:HB	1.88	0.89
1:A:85:LEU:HD22	1:A:87:LEU:HD13	1.53	0.89
1:A:169:LEU:CD1	1:A:169:LEU:C	2.40	0.89
1:A:447:ASP:HA	4:A:818:HOH:O	1.74	0.88
1:A:398:LEU:H	1:A:398:LEU:HD23	1.38	0.88
3:A:802:C8E:C5	3:A:802:C8E:C1	2.38	0.88
1:A:555:VAL:HG12	1:A:556:THR:CG2	2.04	0.88
1:A:495:LEU:O	1:A:496:LEU:HB2	1.71	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:ASN:C	1:A:87:LEU:CD1	2.43	0.87
1:A:174:HIS:CD2	1:A:175:THR:N	2.43	0.87
3:A:802:C8E:C14	3:A:802:C8E:H101	2.04	0.87
1:A:518:MSE:HE1	1:A:547:TRP:CZ3	2.10	0.87
3:A:803:C8E:H112	3:A:803:C8E:H162	1.57	0.86
1:A:10:VAL:HG12	1:A:11:THR:N	1.90	0.85
1:A:174:HIS:HD2	1:A:175:THR:N	1.75	0.84
1:A:426:THR:HG22	1:A:431:TRP:HE1	1.41	0.84
1:A:9:VAL:HG11	1:A:19:ARG:CD	2.05	0.84
1:A:464:VAL:CG1	3:A:804:C8E:H51	2.08	0.84
1:A:13:ASN:C	1:A:13:ASN:HD22	1.80	0.84
1:A:242:THR:CG2	1:A:277:TYR:CE2	2.60	0.83
1:A:426:THR:CG2	1:A:431:TRP:HE1	1.90	0.83
1:A:98:GLN:HE21	1:A:225:ASN:HD22	1.26	0.83
1:A:62:GLN:HE21	1:A:62:GLN:HA	1.42	0.83
1:A:95:ASP:O	1:A:96:LEU:HB2	1.79	0.83
1:A:518:MSE:HG3	1:A:549:LEU:HD12	1.60	0.83
1:A:556:THR:OG1	1:A:557:SER:N	2.08	0.83
1:A:245:LEU:C	1:A:245:LEU:CD2	2.45	0.82
1:A:159:GLN:HA	1:A:160:LEU:HB3	1.60	0.82
1:A:242:THR:HG22	1:A:277:TYR:CE2	2.15	0.82
1:A:174:HIS:CE1	1:A:176:HIS:CE1	2.68	0.82
1:A:342:LEU:HD11	3:A:803:C8E:C5	2.05	0.82
1:A:559:LEU:O	1:A:559:LEU:CD2	2.25	0.82
1:A:174:HIS:CE1	1:A:176:HIS:CD2	2.68	0.82
1:A:511:LEU:CD1	1:A:511:LEU:N	2.43	0.82
1:A:518:MSE:HE1	1:A:547:TRP:HZ3	1.41	0.81
1:A:13:ASN:ND2	1:A:15:PHE:H	1.77	0.81
1:A:89:GLY:HA3	1:A:91:SER:CA	2.11	0.81
1:A:406:GLY:CA	1:A:452:LYS:CE	2.58	0.81
1:A:174:HIS:CD2	1:A:175:THR:O	2.33	0.81
1:A:174:HIS:HD2	1:A:174:HIS:C	1.82	0.80
1:A:509:TRP:NE1	1:A:511:LEU:HD11	1.97	0.80
1:A:10:VAL:O	1:A:12:ALA:N	2.15	0.80
1:A:13:ASN:C	1:A:13:ASN:ND2	2.35	0.80
1:A:88:ALA:O	1:A:92:GLY:CA	2.30	0.80
1:A:358:ARG:O	3:A:800:C8E:C7	2.29	0.79
1:A:509:TRP:CD1	1:A:511:LEU:HD11	2.17	0.79
1:A:151:ASN:C	1:A:152:TYR:HD2	1.85	0.79
3:A:802:C8E:H101	3:A:802:C8E:H142	1.64	0.79
1:A:153:ASP:OD1	1:A:154:VAL:N	2.16	0.79
1:A:244:LYS:NZ	1:A:246:TYR:HB2	1.98	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:SER:CB	1:A:393:TYR:CZ	2.65	0.79
3:A:802:C8E:C14	3:A:802:C8E:C10	2.61	0.79
1:A:362:ASN:ND2	1:A:365:PHE:H	1.79	0.79
1:A:98:GLN:NE2	1:A:225:ASN:HD22	1.80	0.78
1:A:559:LEU:C	1:A:559:LEU:CD2	2.49	0.78
1:A:358:ARG:C	3:A:800:C8E:C7	2.51	0.78
1:A:245:LEU:HD22	1:A:246:TYR:N	1.97	0.78
1:A:406:GLY:HA3	1:A:452:LYS:HE2	1.66	0.78
1:A:406:GLY:HA3	1:A:452:LYS:HE3	1.59	0.78
1:A:62:GLN:NE2	1:A:62:GLN:HA	1.96	0.78
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.65	0.78
1:A:558:HIS:HB2	1:A:593:THR:O	1.84	0.78
1:A:405:TYR:CD2	1:A:451:LEU:HD13	2.19	0.77
1:A:370:THR:H	3:A:800:C8E:H81	1.50	0.77
1:A:555:VAL:HB	1:A:559:LEU:HD13	1.67	0.77
1:A:405:TYR:CD2	1:A:451:LEU:CD1	2.68	0.77
1:A:147:ASN:C	1:A:148:SER:OG	2.23	0.77
1:A:570:ASP:HB2	1:A:584:ARG:HE	1.50	0.77
1:A:569:PHE:N	1:A:569:PHE:CD1	2.52	0.76
1:A:206:LEU:HB2	1:A:218:VAL:CG2	2.16	0.76
1:A:53:ASP:HB3	1:A:502:GLN:HE22	1.49	0.76
1:A:558:HIS:CB	1:A:593:THR:O	2.34	0.76
1:A:569:PHE:HD1	1:A:569:PHE:N	1.83	0.76
3:A:803:C8E:H202	3:A:803:C8E:H32	1.67	0.76
1:A:131:THR:O	1:A:131:THR:OG1	2.02	0.76
1:A:407:ASN:C	1:A:407:ASN:HD22	1.88	0.76
1:A:527:TYR:CE1	1:A:540:LYS:HG3	2.20	0.76
1:A:488:ASN:CG	1:A:491:THR:HG22	2.06	0.75
1:A:224:ASP:CG	1:A:226:ARG:HH21	1.90	0.75
1:A:159:GLN:HA	1:A:160:LEU:CB	2.16	0.75
1:A:160:LEU:HD23	1:A:166:VAL:CG2	2.17	0.75
1:A:26:THR:HG22	1:A:110:ILE:HG23	1.68	0.75
1:A:358:ARG:O	3:A:800:C8E:H82	1.83	0.75
1:A:245:LEU:CD2	1:A:246:TYR:O	2.35	0.74
1:A:571:LYS:HE2	1:A:572:ASP:O	1.87	0.74
1:A:263:SER:CB	1:A:302:ASN:ND2	2.50	0.74
1:A:447:ASP:OD1	4:A:870:HOH:O	2.04	0.74
1:A:85:LEU:C	1:A:85:LEU:CD2	2.55	0.74
1:A:342:LEU:HD11	3:A:803:C8E:H21	1.68	0.74
1:A:144:TRP:C	1:A:144:TRP:CD1	2.61	0.74
3:A:804:C8E:C7	3:A:804:C8E:H32	2.17	0.74
1:A:242:THR:HG22	1:A:277:TYR:CZ	2.22	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:405:TYR:HD2	1:A:451:LEU:HD13	1.53	0.73
1:A:445:ASP:N	1:A:445:ASP:OD1	2.21	0.73
1:A:407:ASN:HD22	1:A:408:PRO:N	1.87	0.73
1:A:31:ARG:NH1	1:A:35:ASP:OD1	2.20	0.73
1:A:242:THR:HG21	1:A:277:TYR:HH	1.54	0.73
3:A:802:C8E:C10	3:A:802:C8E:H142	2.19	0.73
1:A:42:VAL:HG11	1:A:96:LEU:HD13	1.71	0.73
1:A:77:LEU:HD13	1:A:121:ASP:HB3	1.70	0.72
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.71	0.72
1:A:18:PRO:C	1:A:21:THR:HG22	2.02	0.72
1:A:174:HIS:NE2	1:A:176:HIS:CD2	2.57	0.72
1:A:13:ASN:HD22	1:A:15:PHE:H	1.36	0.71
1:A:245:LEU:HD21	1:A:246:TYR:O	1.90	0.71
1:A:358:ARG:C	3:A:800:C8E:H72	2.10	0.71
1:A:583:GLY:O	1:A:584:ARG:HB2	1.90	0.71
1:A:400:GLN:O	1:A:406:GLY:O	2.09	0.71
1:A:526:ARG:HD2	4:A:872:HOH:O	1.89	0.71
1:A:407:ASN:HD22	1:A:408:PRO:CD	2.03	0.70
1:A:495:LEU:O	1:A:496:LEU:CB	2.39	0.70
1:A:88:ALA:CB	1:A:293:MSE:HE1	2.21	0.70
3:A:802:C8E:H52	3:A:802:C8E:H12	0.74	0.70
1:A:487:ARG:NH1	1:A:492:ASP:O	2.24	0.70
3:A:803:C8E:H82	3:A:805:C8E:H11	1.74	0.70
1:A:567:ASN:HA	4:A:814:HOH:O	1.91	0.70
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.73	0.70
3:A:804:C8E:H32	3:A:804:C8E:H71	1.73	0.70
1:A:511:LEU:N	1:A:511:LEU:HD12	2.05	0.70
1:A:120:SER:HB3	1:A:393:TYR:CZ	2.27	0.69
3:A:805:C8E:H202	4:A:832:HOH:O	1.92	0.69
1:A:245:LEU:C	1:A:245:LEU:HD22	2.12	0.69
1:A:588:LEU:HD13	1:A:589:SER:N	2.07	0.69
1:A:263:SER:CB	1:A:302:ASN:HD22	2.01	0.69
1:A:174:HIS:HD2	1:A:175:THR:CA	2.05	0.69
1:A:407:ASN:ND2	1:A:409:ASN:H	1.91	0.69
1:A:85:LEU:O	1:A:87:LEU:HD13	1.93	0.68
1:A:413:GLU:HG2	1:A:443:LEU:HA	1.74	0.68
1:A:175:THR:O	1:A:176:HIS:CB	2.42	0.68
1:A:226:ARG:NH2	1:A:244:LYS:HE2	2.03	0.68
1:A:197:PHE:CD2	1:A:227:THR:OG1	2.46	0.68
1:A:174:HIS:NE2	1:A:175:THR:O	2.27	0.68
1:A:448:ASP:O	1:A:449:HIS:HB2	1.94	0.68
1:A:83:VAL:HG12	1:A:83:VAL:O	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:ASP:HB3	1:A:502:GLN:NE2	2.08	0.68
1:A:198:LEU:HD12	1:A:199:SER:CA	2.24	0.67
1:A:397:ASN:OD1	1:A:400:GLN:HG3	1.94	0.67
1:A:411:ASP:H	1:A:455:ASN:HD21	1.42	0.67
1:A:405:TYR:HD2	1:A:451:LEU:CD1	2.06	0.67
1:A:564:LYS:HG2	1:A:565:ILE:N	2.09	0.67
1:A:463:GLY:O	3:A:804:C8E:H191	1.95	0.67
1:A:311:ILE:HG22	1:A:311:ILE:O	1.93	0.67
1:A:405:TYR:CE2	1:A:451:LEU:CD1	2.78	0.67
1:A:19:ARG:HB3	1:A:19:ARG:HH11	1.58	0.66
1:A:74:SER:HA	1:A:93:SER:HB2	1.75	0.66
1:A:506:GLN:HE22	1:A:519:THR:CG2	2.07	0.66
1:A:242:THR:CG2	1:A:277:TYR:CE1	2.78	0.66
1:A:568:LEU:HB3	1:A:569:PHE:CE1	2.31	0.66
1:A:531:TYR:O	1:A:533:SER:N	2.29	0.66
1:A:89:GLY:HA2	1:A:92:GLY:CA	2.26	0.66
1:A:527:TYR:CD1	1:A:540:LYS:HG3	2.30	0.65
1:A:44:ASP:OD1	1:A:47:ARG:NH1	2.29	0.65
1:A:407:ASN:ND2	1:A:407:ASN:C	2.48	0.65
1:A:43:ASN:N	4:A:866:HOH:O	2.19	0.65
1:A:175:THR:O	1:A:176:HIS:HB2	1.96	0.65
3:A:803:C8E:H82	3:A:805:C8E:C1	2.26	0.65
1:A:518:MSE:CE	1:A:547:TRP:CZ3	2.80	0.65
1:A:206:LEU:CB	1:A:218:VAL:CG2	2.75	0.65
1:A:358:ARG:O	3:A:800:C8E:H81	1.95	0.65
1:A:151:ASN:O	1:A:152:TYR:HD2	1.79	0.65
1:A:558:HIS:N	1:A:558:HIS:ND1	2.45	0.65
1:A:174:HIS:HE1	1:A:176:HIS:CE1	2.14	0.65
1:A:509:TRP:CD1	1:A:511:LEU:CD1	2.79	0.64
1:A:52:VAL:HG12	1:A:52:VAL:O	1.97	0.64
1:A:245:LEU:HD23	1:A:273:LYS:O	1.98	0.64
3:A:802:C8E:H172	3:A:802:C8E:H11	1.79	0.64
1:A:77:LEU:HD21	1:A:79:LEU:HD21	1.79	0.63
1:A:242:THR:HG21	1:A:277:TYR:CE1	2.26	0.63
1:A:244:LYS:HZ2	1:A:246:TYR:HB2	1.64	0.63
1:A:144:TRP:HD1	1:A:144:TRP:O	1.81	0.63
1:A:159:GLN:HB3	1:A:164:THR:O	1.97	0.63
1:A:527:TYR:HE1	1:A:540:LYS:CG	2.09	0.63
1:A:174:HIS:CD2	1:A:175:THR:C	2.72	0.63
1:A:82:GLY:HA2	1:A:83:VAL:CB	2.29	0.63
1:A:398:LEU:N	1:A:398:LEU:CD2	2.52	0.62
1:A:89:GLY:HA2	1:A:92:GLY:HA2	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:LEU:HD13	1:A:199:SER:N	2.14	0.62
1:A:13:ASN:ND2	1:A:15:PHE:N	2.46	0.62
1:A:82:GLY:HA2	1:A:83:VAL:HB	1.80	0.62
1:A:506:GLN:HE21	1:A:519:THR:HB	1.64	0.62
1:A:151:ASN:O	1:A:152:TYR:CD2	2.52	0.62
1:A:518:MSE:HG3	1:A:549:LEU:HD13	1.81	0.62
1:A:45:VAL:O	1:A:46:LEU:HG	2.00	0.62
1:A:164:THR:OG1	1:A:208:HIS:HD2	1.83	0.61
1:A:506:GLN:HE22	1:A:519:THR:CB	2.13	0.61
1:A:82:GLY:HA2	1:A:83:VAL:O	2.00	0.61
1:A:495:LEU:O	1:A:496:LEU:CD1	2.48	0.61
1:A:120:SER:HB3	1:A:393:TYR:CE1	2.33	0.60
1:A:398:LEU:H	1:A:398:LEU:HD22	1.66	0.60
1:A:68:ILE:O	1:A:71:THR:HG23	2.01	0.60
1:A:334:ASP:OD2	1:A:336:ARG:NH2	2.33	0.60
1:A:245:LEU:CD2	1:A:246:TYR:C	2.69	0.60
1:A:87:LEU:N	1:A:87:LEU:CD1	2.65	0.60
1:A:405:TYR:HE2	1:A:451:LEU:HD11	1.66	0.60
1:A:506:GLN:NE2	1:A:519:THR:CB	2.63	0.60
1:A:57:ASN:HB3	1:A:579:TYR:CD2	2.36	0.60
1:A:103:LEU:HD21	1:A:201:THR:HG21	1.83	0.60
1:A:31:ARG:O	1:A:34:ILE:N	2.35	0.60
1:A:406:GLY:HA2	1:A:452:LYS:HE3	1.80	0.60
1:A:113:PRO:HD3	1:A:417:GLN:CD	2.21	0.60
3:A:803:C8E:C11	3:A:803:C8E:H162	2.29	0.60
1:A:534:TYR:HA	1:A:535:PRO:C	2.22	0.60
1:A:224:ASP:C	1:A:224:ASP:OD1	2.39	0.59
1:A:198:LEU:O	1:A:198:LEU:HD12	2.00	0.59
3:A:805:C8E:H161	3:A:805:C8E:O21	2.03	0.59
1:A:324:PRO:C	1:A:326:THR:H	2.05	0.59
1:A:529:LYS:NZ	1:A:538:THR:HG22	2.17	0.59
1:A:102:ALA:C	1:A:103:LEU:HD23	2.22	0.59
1:A:87:LEU:N	1:A:87:LEU:HD12	2.15	0.59
1:A:17:GLN:HG3	1:A:21:THR:CG2	2.33	0.58
1:A:98:GLN:NE2	4:A:823:HOH:O	2.36	0.58
1:A:47:ARG:HG3	1:A:48:ARG:N	2.18	0.58
1:A:511:LEU:N	1:A:511:LEU:HD13	2.19	0.58
1:A:224:ASP:OD2	1:A:226:ARG:NH2	2.35	0.58
1:A:175:THR:O	1:A:176:HIS:CG	2.56	0.58
1:A:13:ASN:O	1:A:14:ARG:HB2	2.03	0.58
1:A:85:LEU:C	1:A:87:LEU:H	2.06	0.58
1:A:88:ALA:HB3	1:A:293:MSE:HE1	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:362:ASN:CG	1:A:365:PHE:CE2	2.77	0.58
1:A:491:THR:HG23	1:A:493:THR:HG23	1.85	0.58
1:A:553:TYR:CE2	1:A:555:VAL:HG22	2.39	0.57
1:A:296:TYR:HE1	1:A:321:MSE:CG	2.17	0.57
1:A:85:LEU:C	1:A:87:LEU:N	2.56	0.57
1:A:436:TYR:O	3:A:804:C8E:H202	2.04	0.57
1:A:447:ASP:O	1:A:448:ASP:HB2	2.04	0.57
1:A:116:ALA:HA	1:A:370:THR:CG2	2.34	0.57
3:A:804:C8E:C3	3:A:804:C8E:H71	2.35	0.57
1:A:89:GLY:CA	1:A:92:GLY:HA2	2.33	0.57
1:A:405:TYR:CE2	1:A:451:LEU:HD11	2.40	0.57
1:A:495:LEU:O	1:A:496:LEU:HD13	2.05	0.57
1:A:534:TYR:CG	1:A:535:PRO:HA	2.39	0.57
1:A:553:TYR:HD2	1:A:555:VAL:CG2	2.18	0.57
1:A:323:THR:HG23	1:A:324:PRO:CD	2.35	0.57
1:A:116:ALA:HA	1:A:370:THR:HG22	1.87	0.57
1:A:53:ASP:C	1:A:53:ASP:OD1	2.43	0.57
1:A:553:TYR:HD2	1:A:555:VAL:HG23	1.70	0.56
1:A:567:ASN:C	4:A:814:HOH:O	2.44	0.56
1:A:518:MSE:CE	1:A:547:TRP:CE3	2.88	0.56
1:A:592:TYR:CE1	1:A:594:PHE:HB3	2.41	0.56
1:A:518:MSE:HE3	1:A:547:TRP:CE3	2.40	0.56
1:A:502:GLN:HG2	1:A:523:LEU:HD22	1.86	0.56
1:A:160:LEU:CD2	1:A:166:VAL:HG23	2.35	0.56
1:A:52:VAL:HG22	1:A:68:ILE:HD13	1.87	0.56
1:A:82:GLY:HA2	1:A:83:VAL:C	2.26	0.56
1:A:567:ASN:ND2	1:A:571:LYS:H	2.03	0.56
1:A:113:PRO:HD3	1:A:417:GLN:NE2	2.20	0.56
1:A:120:SER:HB2	1:A:393:TYR:CD1	2.35	0.56
1:A:406:GLY:HA3	1:A:407:ASN:HB2	1.88	0.56
1:A:7:THR:O	1:A:7:THR:HG22	2.05	0.56
1:A:491:THR:HG23	1:A:493:THR:H	1.71	0.56
1:A:433:ILE:HD12	3:A:802:C8E:H13	1.88	0.56
1:A:568:LEU:O	1:A:584:ARG:NH2	2.39	0.56
1:A:86:ASN:O	1:A:87:LEU:CD1	2.27	0.55
1:A:205:ALA:O	1:A:206:LEU:HD12	2.06	0.55
1:A:218:VAL:HG23	1:A:218:VAL:O	2.05	0.55
1:A:10:VAL:N	1:A:108:GLU:OE1	2.39	0.55
1:A:323:THR:O	1:A:326:THR:OG1	2.24	0.55
1:A:13:ASN:HD21	1:A:15:PHE:HB2	1.70	0.55
1:A:558:HIS:O	1:A:559:LEU:HB2	2.07	0.55
1:A:407:ASN:HB2	1:A:452:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:ARG:HH12	1:A:244:LYS:CD	2.19	0.55
1:A:464:VAL:CG2	3:A:804:C8E:C5	2.84	0.55
1:A:18:PRO:CD	1:A:21:THR:HG21	2.30	0.55
1:A:144:TRP:O	1:A:144:TRP:CD1	2.58	0.55
1:A:52:VAL:HG22	1:A:68:ILE:CD1	2.36	0.55
1:A:436:TYR:C	3:A:804:C8E:H202	2.27	0.55
1:A:506:GLN:HE22	1:A:519:THR:HB	1.65	0.55
1:A:562:ARG:O	1:A:588:LEU:HD22	2.07	0.55
1:A:460:ARG:HE	1:A:462:LYS:HE3	1.71	0.55
1:A:226:ARG:NH1	1:A:244:LYS:CG	2.38	0.55
1:A:436:TYR:O	3:A:804:C8E:C20	2.56	0.54
1:A:153:ASP:HB2	1:A:171:ASP:OD1	2.06	0.54
1:A:80:ILE:O	1:A:83:VAL:CG1	2.55	0.54
1:A:407:ASN:HD22	1:A:408:PRO:HD2	1.72	0.54
1:A:529:LYS:HZ3	1:A:538:THR:HG22	1.72	0.54
1:A:477:HIS:CE1	1:A:507:LEU:HD11	2.42	0.54
1:A:165:ARG:HG2	1:A:207:GLU:HB2	1.89	0.54
1:A:226:ARG:CZ	1:A:244:LYS:HG3	2.29	0.54
1:A:206:LEU:HB2	1:A:218:VAL:HG21	1.88	0.54
1:A:75:HIS:O	1:A:123:ILE:O	2.26	0.54
1:A:579:TYR:N	1:A:579:TYR:CD1	2.76	0.54
1:A:588:LEU:HD13	1:A:588:LEU:C	2.26	0.54
1:A:373:THR:HG23	3:A:803:C8E:H102	1.89	0.54
1:A:358:ARG:N	3:A:800:C8E:H71	2.23	0.54
1:A:362:ASN:ND2	1:A:365:PHE:CE2	2.76	0.54
1:A:120:SER:HB3	1:A:393:TYR:OH	2.09	0.53
1:A:557:SER:HB3	1:A:558:HIS:CE1	2.42	0.53
1:A:166:VAL:HG13	1:A:206:LEU:CD1	2.38	0.53
1:A:40:THR:O	1:A:41:SER:CB	2.55	0.53
1:A:527:TYR:HE1	1:A:540:LYS:CD	2.22	0.53
1:A:21:THR:OG1	1:A:345:LEU:HD11	2.08	0.53
1:A:464:VAL:CG2	3:A:804:C8E:H51	2.39	0.53
1:A:296:TYR:HE1	1:A:321:MSE:HG3	1.72	0.53
1:A:380:ILE:O	1:A:381:GLU:C	2.46	0.53
1:A:558:HIS:O	1:A:592:TYR:CD2	2.60	0.53
1:A:69:ARG:HD3	1:A:436:TYR:CZ	2.43	0.53
1:A:24:ALA:HB2	4:A:856:HOH:O	2.07	0.53
1:A:18:PRO:HD2	1:A:21:THR:CG2	2.31	0.53
1:A:367:ARG:HH21	3:A:800:C8E:H172	1.72	0.53
1:A:153:ASP:OD1	1:A:153:ASP:C	2.45	0.53
1:A:553:TYR:CD2	1:A:555:VAL:HG22	2.43	0.53
1:A:342:LEU:HD12	1:A:342:LEU:C	2.29	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:LEU:HD11	1:A:200:LYS:HG3	1.90	0.52
1:A:567:ASN:CA	4:A:814:HOH:O	2.53	0.52
1:A:527:TYR:CE1	1:A:540:LYS:HD2	2.44	0.52
1:A:438:ASN:C	1:A:438:ASN:OD1	2.47	0.52
1:A:11:THR:O	1:A:118:TYR:OH	2.18	0.52
1:A:553:TYR:CD2	1:A:555:VAL:CG2	2.93	0.52
1:A:592:TYR:HE1	1:A:594:PHE:CG	2.28	0.52
1:A:98:GLN:HE22	1:A:225:ASN:CB	2.23	0.52
1:A:88:ALA:HB3	1:A:293:MSE:CE	2.40	0.52
1:A:10:VAL:O	1:A:11:THR:C	2.48	0.52
1:A:74:SER:CA	1:A:93:SER:HB2	2.39	0.51
1:A:89:GLY:CA	1:A:90:VAL:C	2.38	0.51
1:A:400:GLN:O	1:A:407:ASN:N	2.43	0.51
1:A:98:GLN:HE22	1:A:225:ASN:HB3	1.75	0.51
1:A:261:ILE:HG12	1:A:304:VAL:CG1	2.40	0.51
1:A:458:LYS:HD2	1:A:490:ILE:HD11	1.91	0.51
1:A:138:THR:HG22	1:A:156:THR:OG1	2.09	0.51
1:A:174:HIS:HB2	1:A:198:LEU:HA	1.93	0.51
1:A:319:MSE:HG3	1:A:336:ARG:HG2	1.92	0.51
1:A:157:GLN:HB2	1:A:167:THR:HG23	1.91	0.51
1:A:531:TYR:O	1:A:532:SER:C	2.48	0.51
1:A:206:LEU:HB2	1:A:218:VAL:HG23	1.90	0.51
1:A:45:VAL:O	1:A:46:LEU:CG	2.59	0.51
1:A:140:ILE:HG12	1:A:154:VAL:HG22	1.92	0.51
1:A:49:LEU:HB3	1:A:50:PRO:HD2	1.93	0.51
1:A:527:TYR:HE1	1:A:540:LYS:HD2	1.77	0.50
1:A:464:VAL:HG21	3:A:804:C8E:C5	2.41	0.50
1:A:513:ASP:O	1:A:554:PRO:HD2	2.11	0.50
1:A:81:ASP:OD2	1:A:131:THR:HG23	2.12	0.50
1:A:245:LEU:HD22	1:A:246:TYR:C	2.32	0.50
1:A:151:ASN:C	1:A:152:TYR:CD2	2.75	0.50
1:A:567:ASN:HD21	1:A:571:LYS:H	1.58	0.50
1:A:488:ASN:CB	1:A:491:THR:HG22	2.42	0.50
1:A:226:ARG:NH1	1:A:226:ARG:HG3	2.26	0.50
1:A:85:LEU:CD2	1:A:87:LEU:HD13	2.32	0.50
1:A:555:VAL:O	1:A:556:THR:CB	2.58	0.50
1:A:80:ILE:O	1:A:83:VAL:HG12	2.12	0.50
1:A:68:ILE:HG13	1:A:76:VAL:CG2	2.42	0.50
1:A:89:GLY:CA	1:A:91:SER:H	2.05	0.50
1:A:534:TYR:C	1:A:534:TYR:CD1	2.85	0.50
1:A:451:LEU:O	1:A:452:LYS:HG2	2.11	0.49
1:A:398:LEU:N	1:A:398:LEU:HD22	2.22	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:559:LEU:HA	1:A:591:SER:O	2.12	0.49
1:A:241:ASP:N	1:A:241:ASP:OD2	2.45	0.49
1:A:370:THR:H	3:A:800:C8E:C8	2.21	0.49
3:A:805:C8E:H161	3:A:805:C8E:C20	2.32	0.49
1:A:406:GLY:N	1:A:452:LYS:HE3	2.27	0.49
1:A:7:THR:CG2	1:A:7:THR:O	2.61	0.49
1:A:506:GLN:HE22	1:A:519:THR:HG22	1.75	0.49
1:A:422:PHE:CD2	3:A:801:C8E:H11	2.48	0.49
1:A:373:THR:HG21	3:A:803:C8E:H131	1.94	0.49
1:A:568:LEU:N	4:A:814:HOH:O	2.46	0.49
1:A:414:LYS:HE3	1:A:442:ASP:OD1	2.12	0.49
1:A:19:ARG:C	1:A:21:THR:H	2.15	0.49
1:A:25:PRO:C	1:A:26:THR:CG2	2.81	0.49
1:A:23:LEU:O	1:A:24:ALA:HB2	2.12	0.49
1:A:102:ALA:C	1:A:103:LEU:CD2	2.79	0.49
1:A:70:GLY:CA	1:A:484:VAL:HG11	2.43	0.48
1:A:371:TRP:H	1:A:391:THR:HG22	1.77	0.48
3:A:803:C8E:H202	3:A:803:C8E:C3	2.39	0.48
1:A:445:ASP:O	1:A:453:TYR:HD1	1.97	0.48
1:A:46:LEU:O	1:A:52:VAL:HG11	2.14	0.48
1:A:464:VAL:HG13	3:A:804:C8E:C4	2.43	0.48
1:A:464:VAL:HG21	3:A:804:C8E:H51	1.95	0.48
1:A:275:TYR:CZ	1:A:290:LEU:HD13	2.48	0.48
1:A:426:THR:CG2	1:A:431:TRP:NE1	2.69	0.48
1:A:197:PHE:HD2	1:A:227:THR:OG1	1.93	0.48
1:A:573:TYR:CE1	1:A:581:THR:HG21	2.49	0.48
1:A:89:GLY:HA2	1:A:92:GLY:N	2.29	0.48
1:A:79:LEU:HA	1:A:84:ARG:HA	1.95	0.48
1:A:19:ARG:C	1:A:21:THR:N	2.67	0.48
3:A:805:C8E:H142	3:A:805:C8E:H172	1.41	0.48
1:A:63:LEU:N	1:A:63:LEU:HD23	2.29	0.47
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.56	0.47
1:A:85:LEU:O	1:A:86:ASN:C	2.48	0.47
1:A:370:THR:HB	4:A:839:HOH:O	2.13	0.47
1:A:53:ASP:O	1:A:53:ASP:OD1	2.31	0.47
1:A:70:GLY:HA3	1:A:484:VAL:HG11	1.95	0.47
1:A:512:TYR:CD2	1:A:512:TYR:N	2.82	0.47
1:A:44:ASP:HA	1:A:47:ARG:HD3	1.95	0.47
1:A:77:LEU:CD1	1:A:121:ASP:HB3	2.43	0.47
1:A:319:MSE:CG	1:A:336:ARG:HG2	2.44	0.47
1:A:147:ASN:HA	1:A:147:ASN:HD22	1.51	0.47
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:HIS:CD2	1:A:174:HIS:O	2.68	0.47
1:A:269:TYR:HA	1:A:295:GLN:O	2.14	0.47
1:A:159:GLN:CA	1:A:160:LEU:CB	2.88	0.47
1:A:98:GLN:NE2	1:A:225:ASN:CB	2.78	0.47
1:A:275:TYR:CE2	1:A:290:LEU:HD13	2.49	0.47
1:A:72:ASN:OD1	1:A:498:ARG:NH2	2.41	0.47
1:A:451:LEU:C	1:A:452:LYS:CG	2.83	0.46
1:A:322:THR:HG22	1:A:326:THR:HG21	1.97	0.46
1:A:342:LEU:CD1	3:A:803:C8E:H21	2.42	0.46
1:A:319:MSE:HG2	1:A:336:ARG:HG3	1.97	0.46
1:A:323:THR:HG22	1:A:326:THR:OG1	2.16	0.46
1:A:13:ASN:ND2	1:A:13:ASN:O	2.49	0.46
1:A:151:ASN:OD1	1:A:151:ASN:C	2.53	0.46
1:A:245:LEU:HD22	1:A:246:TYR:CA	2.46	0.46
1:A:80:ILE:HD13	1:A:129:ILE:HB	1.96	0.46
1:A:523:LEU:HA	1:A:523:LEU:HD22	1.68	0.46
1:A:49:LEU:HB3	1:A:50:PRO:CD	2.46	0.46
1:A:383:TYR:OH	1:A:426:THR:HB	2.16	0.46
1:A:17:GLN:HG3	1:A:21:THR:HG21	1.97	0.46
1:A:132:THR:HG22	1:A:133:ARG:N	2.31	0.46
3:A:800:C8E:H141	3:A:800:C8E:H112	1.37	0.46
1:A:423:GLU:HB2	1:A:432:ARG:HG3	1.98	0.45
1:A:559:LEU:O	1:A:559:LEU:CG	2.63	0.45
1:A:17:GLN:HE21	1:A:21:THR:HG23	1.81	0.45
1:A:426:THR:O	1:A:427:ALA:C	2.55	0.45
1:A:323:THR:CG2	1:A:324:PRO:N	2.78	0.45
1:A:541:MSE:CE	1:A:574:GLU:HB2	2.46	0.45
1:A:379:PHE:O	1:A:380:ILE:HG13	2.15	0.45
1:A:17:GLN:HE21	1:A:22:VAL:HG22	1.82	0.45
3:A:802:C8E:H101	3:A:802:C8E:H141	1.95	0.45
1:A:245:LEU:CD2	1:A:246:TYR:CA	2.94	0.45
1:A:511:LEU:HB3	1:A:512:TYR:CD2	2.51	0.45
1:A:8:LEU:HD23	1:A:16:GLU:OE2	2.16	0.45
1:A:359:SER:HB2	3:A:800:C8E:H72	1.98	0.45
1:A:146:SER:O	1:A:147:ASN:HB2	2.17	0.45
1:A:558:HIS:HB3	1:A:593:THR:O	2.16	0.45
1:A:82:GLY:CA	1:A:83:VAL:HB	2.47	0.45
3:A:802:C8E:H102	3:A:802:C8E:H142	1.96	0.44
1:A:576:VAL:O	1:A:579:TYR:HD1	2.01	0.44
1:A:358:ARG:CA	3:A:800:C8E:H71	2.48	0.44
1:A:527:TYR:CE1	1:A:540:LYS:CD	3.01	0.44
1:A:353:PHE:HB3	3:A:803:C8E:H171	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:496:LEU:HD21	1:A:529:LYS:HG3	1.98	0.44
1:A:470:PHE:CE1	1:A:477:HIS:CG	3.05	0.44
1:A:400:GLN:O	1:A:406:GLY:C	2.55	0.44
1:A:529:LYS:NZ	1:A:538:THR:CG2	2.80	0.44
1:A:448:ASP:O	1:A:449:HIS:CB	2.62	0.44
1:A:510:GLN:C	1:A:511:LEU:HD12	2.37	0.44
1:A:422:PHE:CG	3:A:801:C8E:H11	2.53	0.44
1:A:159:GLN:HG2	1:A:159:GLN:H	1.62	0.44
1:A:164:THR:OG1	1:A:208:HIS:CD2	2.67	0.44
1:A:324:PRO:C	1:A:326:THR:N	2.70	0.44
1:A:588:LEU:HD22	1:A:588:LEU:HA	1.50	0.43
1:A:555:VAL:HG12	1:A:556:THR:HG23	1.96	0.43
1:A:319:MSE:HG2	1:A:336:ARG:CG	2.48	0.43
1:A:323:THR:HG23	1:A:324:PRO:N	2.32	0.43
1:A:349:GLY:O	1:A:351:PHE:N	2.51	0.43
1:A:584:ARG:HD3	1:A:584:ARG:HA	1.21	0.43
1:A:265:LEU:C	1:A:266:ILE:HG13	2.37	0.43
1:A:349:GLY:O	1:A:351:PHE:HD1	2.01	0.43
1:A:43:ASN:CG	4:A:866:HOH:O	2.56	0.43
1:A:406:GLY:HA3	1:A:407:ASN:CB	2.49	0.43
1:A:291:ASP:HA	1:A:326:THR:HG23	2.00	0.43
1:A:99:PHE:HA	1:A:100:PRO:HD3	1.72	0.43
1:A:169:LEU:CD1	1:A:170:GLY:N	2.81	0.43
1:A:360:ASP:O	1:A:367:ARG:HA	2.19	0.43
1:A:541:MSE:HE2	1:A:574:GLU:O	2.18	0.43
1:A:103:LEU:HD23	1:A:103:LEU:H	1.71	0.42
1:A:88:ALA:HB2	1:A:320:GLN:OE1	2.19	0.42
1:A:342:LEU:HD12	1:A:343:THR:N	2.34	0.42
1:A:13:ASN:HD22	1:A:14:ARG:N	2.16	0.42
1:A:105:GLN:OE1	1:A:133:ARG:HD2	2.19	0.42
1:A:460:ARG:NE	1:A:462:LYS:HE3	2.34	0.42
1:A:120:SER:CA	1:A:393:TYR:CZ	3.02	0.42
1:A:402:TYR:HE2	1:A:408:PRO:HB3	1.85	0.42
1:A:261:ILE:HG12	1:A:304:VAL:HG12	2.01	0.42
1:A:221:TYR:C	1:A:221:TYR:CD1	2.92	0.42
1:A:9:VAL:HG13	1:A:19:ARG:HD3	1.84	0.42
1:A:592:TYR:CE1	1:A:594:PHE:CD1	3.08	0.42
1:A:152:TYR:N	1:A:152:TYR:CD2	2.87	0.42
1:A:111:ARG:NH2	1:A:465:GLU:OE2	2.44	0.42
3:A:803:C8E:H71	3:A:803:C8E:H41	1.78	0.42
1:A:116:ALA:CA	1:A:370:THR:CG2	2.98	0.42
1:A:451:LEU:HA	1:A:451:LEU:HD22	1.74	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:GLY:HA3	1:A:228:ASN:HB2	2.02	0.42
1:A:358:ARG:C	3:A:800:C8E:H71	2.37	0.41
1:A:322:THR:HG22	1:A:326:THR:CG2	2.50	0.41
1:A:541:MSE:HE3	1:A:574:GLU:HB2	2.03	0.41
1:A:164:THR:HA	1:A:207:GLU:O	2.20	0.41
1:A:166:VAL:HG13	1:A:206:LEU:HD12	2.02	0.41
1:A:311:ILE:HD11	3:A:803:C8E:C1	2.50	0.41
1:A:377:TRP:CD1	1:A:377:TRP:C	2.89	0.41
1:A:415:SER:HB2	1:A:440:VAL:HG22	2.01	0.41
1:A:404:PHE:O	1:A:404:PHE:HD2	2.04	0.41
1:A:17:GLN:HA	1:A:18:PRO:HD3	1.85	0.41
1:A:98:GLN:NE2	1:A:225:ASN:ND2	2.59	0.41
1:A:23:LEU:HD22	1:A:386:ILE:HD13	2.03	0.41
1:A:267:THR:HG22	1:A:267:THR:O	2.21	0.41
1:A:407:ASN:ND2	1:A:408:PRO:HD2	2.35	0.41
1:A:452:LYS:HB3	1:A:452:LYS:HE2	1.76	0.41
1:A:88:ALA:O	1:A:92:GLY:C	2.59	0.41
1:A:85:LEU:C	1:A:85:LEU:HD23	2.38	0.41
1:A:98:GLN:HE21	1:A:98:GLN:HB3	1.72	0.41
1:A:445:ASP:O	1:A:453:TYR:CD1	2.74	0.41
1:A:123:ILE:HG12	1:A:392:SER:HB2	2.03	0.41
1:A:23:LEU:HD11	1:A:352:THR:HG22	2.01	0.41
1:A:49:LEU:CB	1:A:50:PRO:CD	2.98	0.41
1:A:257:ASN:OD1	1:A:262:LYS:HE2	2.21	0.41
1:A:344:GLY:C	3:A:803:C8E:H191	2.41	0.40
1:A:520:MSE:HG2	1:A:521:GLN:N	2.35	0.40
1:A:530:ASP:OD1	1:A:530:ASP:C	2.59	0.40
1:A:359:SER:N	3:A:800:C8E:H72	2.36	0.40
3:A:805:C8E:C20	4:A:832:HOH:O	2.61	0.40
1:A:160:LEU:HD23	1:A:166:VAL:HG23	1.99	0.40
1:A:451:LEU:C	1:A:452:LYS:HG2	2.41	0.40
1:A:344:GLY:O	3:A:803:C8E:H191	2.22	0.40
1:A:445:ASP:O	1:A:453:TYR:HA	2.21	0.40
1:A:348:VAL:O	1:A:349:GLY:O	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:367:ARG:NH1	1:A:427:ALA:O[6_655]	1.77	0.43

## 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	534/594 (90%)	468 (88%)	46 (9%)	20 (4%)	5 11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	41	SER
1	A	86	ASN
1	A	147	ASN
1	A	449	HIS
1	A	450	THR
1	A	496	LEU
1	A	559	LEU
1	A	584	ARG
1	A	46	LEU
1	A	121	ASP
1	A	349	GLY
1	A	451	LEU
1	A	495	LEU
1	A	532	SER
1	A	556	THR
1	A	83	VAL
1	A	89	GLY
1	A	91	SER
1	A	92	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	453/487 (93%)	367 (81%)	86 (19%)	<b>2</b> <b>6</b>

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	19	ARG
1	A	31	ARG
1	A	49	LEU
1	A	53	ASP
1	A	62	GLN
1	A	65	SER
1	A	84	ARG
1	A	85	LEU
1	A	86	ASN
1	A	91	SER
1	A	103	LEU
1	A	111	ARG
1	A	114	ARG
1	A	115	SER
1	A	120	SER
1	A	121	ASP
1	A	131	THR
1	A	144	TRP
1	A	147	ASN
1	A	148	SER
1	A	151	ASN
1	A	158	GLN
1	A	159	GLN
1	A	163	LYS
1	A	169	LEU
1	A	174	HIS
1	A	198	LEU
1	A	202	LEU
1	A	215	SER
1	A	218	VAL
1	A	224	ASP
1	A	226	ARG
1	A	241	ASP
1	A	242	THR
1	A	245	LEU
1	A	249	SER
1	A	259	GLU

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Mol	Chain	Res	Type
1	A	267	THR
1	A	270	SER
1	A	299	GLN
1	A	304	VAL
1	A	311	ILE
1	A	315	VAL
1	A	322	THR
1	A	323	THR
1	A	338	THR
1	A	340	ILE
1	A	342	LEU
1	A	345	LEU
1	A	346	GLN
1	A	370	THR
1	A	391	THR
1	A	398	LEU
1	A	404	PHE
1	A	407	ASN
1	A	415	SER
1	A	425	LEU
1	A	426	THR
1	A	433	ILE
1	A	445	ASP
1	A	451	LEU
1	A	496	LEU
1	A	507	LEU
1	A	510	GLN
1	A	511	LEU
1	A	512	TYR
1	A	519	THR
1	A	520	MSE
1	A	523	LEU
1	A	526	ARG
1	A	533	SER
1	A	539	VAL
1	A	540	LYS
1	A	544	VAL
1	A	556	THR
1	A	558	HIS
1	A	559	LEU
1	A	567	ASN
1	A	568	LEU

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Mol	Chain	Res	Type
1	A	569	PHE
1	A	571	LYS
1	A	572	ASP
1	A	579	TYR
1	A	584	ARG
1	A	585	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	17	GLN
1	A	32	GLN
1	A	62	GLN
1	A	98	GLN
1	A	147	ASN
1	A	150	GLN
1	A	158	GLN
1	A	174	HIS
1	A	208	HIS
1	A	302	ASN
1	A	337	ASN
1	A	347	GLN
1	A	362	ASN
1	A	372	GLN
1	A	400	GLN
1	A	407	ASN
1	A	417	GLN
1	A	455	ASN
1	A	502	GLN
1	A	506	GLN
1	A	510	GLN
1	A	567	ASN
1	A	580	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 ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	C8E	A	800	1	20,20,20	0.38	0	19,19,19	0.77	0
3	C8E	A	801	-	20,20,20	0.35	0	19,19,19	0.59	0
3	C8E	A	802	-	20,20,20	0.36	0	19,19,19	0.76	1 (5%)
3	C8E	A	803	-	20,20,20	0.43	0	19,19,19	0.69	0
3	C8E	A	804	-	20,20,20	0.36	0	19,19,19	0.51	0
3	C8E	A	805	-	20,20,20	0.41	0	19,19,19	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	800	1	-	0/18/18/18	0/0/0/0
3	C8E	A	801	-	-	0/18/18/18	0/0/0/0
3	C8E	A	802	-	-	0/18/18/18	0/0/0/0
3	C8E	A	803	-	-	0/18/18/18	0/0/0/0
3	C8E	A	804	-	-	0/18/18/18	0/0/0/0
3	C8E	A	805	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	C8E	C10-O9-C8	-2.16	103.87	113.38

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, 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	544/594 (91%)	-0.03	25 (4%) 31 35	18, 37, 64, 102	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	TYR	7.5
1	A	579	TYR	5.5
1	A	288	ALA	5.1
1	A	573	TYR	4.8
1	A	175	THR	3.9
1	A	88	ALA	3.6
1	A	289	THR	3.4
1	A	148	SER	3.4
1	A	196	GLY	3.2
1	A	324	PRO	3.0
1	A	276	ASN	3.0
1	A	511	LEU	2.9
1	A	241	ASP	2.8
1	A	176	HIS	2.8
1	A	512	TYR	2.7
1	A	275	TYR	2.6
1	A	404	PHE	2.6
1	A	160	LEU	2.4
1	A	325	GLY	2.4
1	A	594	PHE	2.3
1	A	580	GLN	2.3
1	A	242	THR	2.2
1	A	144	TRP	2.1
1	A	162	ASP	2.0
1	A	582	ALA	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	C8E	A	802	21/21	0.30	5.00	47,57,93,103	0
3	C8E	A	803	21/21	0.29	4.75	57,79,114,123	0
3	C8E	A	805	21/21	0.33	4.33	41,85,184,197	0
3	C8E	A	801	21/21	0.28	3.68	39,66,118,123	0
3	C8E	A	804	21/21	0.22	2.69	32,55,95,98	0
3	C8E	A	800	21/21	0.21	1.10	29,62,92,116	0
2	MG	A	806	1/1	0.14	-1.72	73,73,73,73	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.