



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3NAM  
Title : SR Ca(2+)-ATPase in the HnE2 state complexed with the Thapsigargin derivative dOTg  
Authors : Winther, A.M.L.; Sonntag, Y.; Olesen, C.; Moller, J.V.; Nissen, P.  
Deposited on : 2010-06-02  
Resolution : 3.10 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

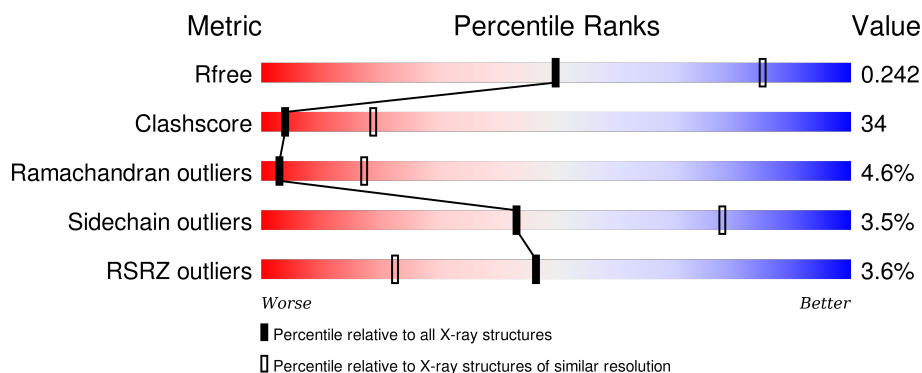
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	994	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OTK	A	997	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7736 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 SERCA1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

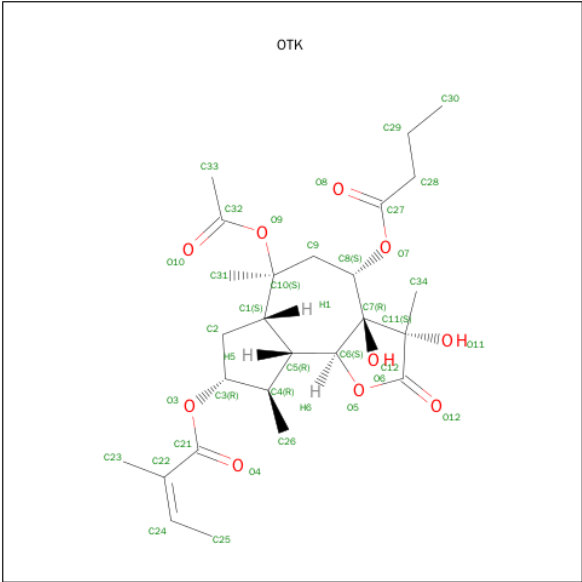
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

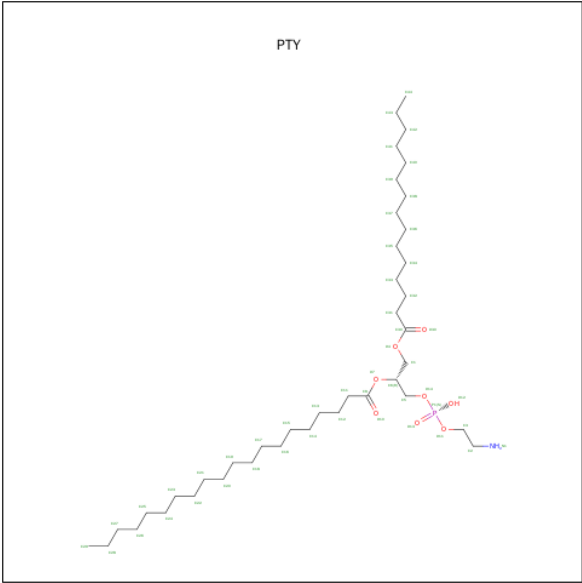
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (3S,3AR,4S,6S,6AS,8R,9R,9AR,9BS)-6-(ACETYLOXY)-4-(BUTANOYL OXY)-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-2-OXODECAHYDROAZULENO[4,5-B]FURAN-8-YL (2Z)-2-METHYLBUT-2-ENOATE (three-letter code: OTK) (formula: C<sub>26</sub>H<sub>38</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			36	26	10		

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

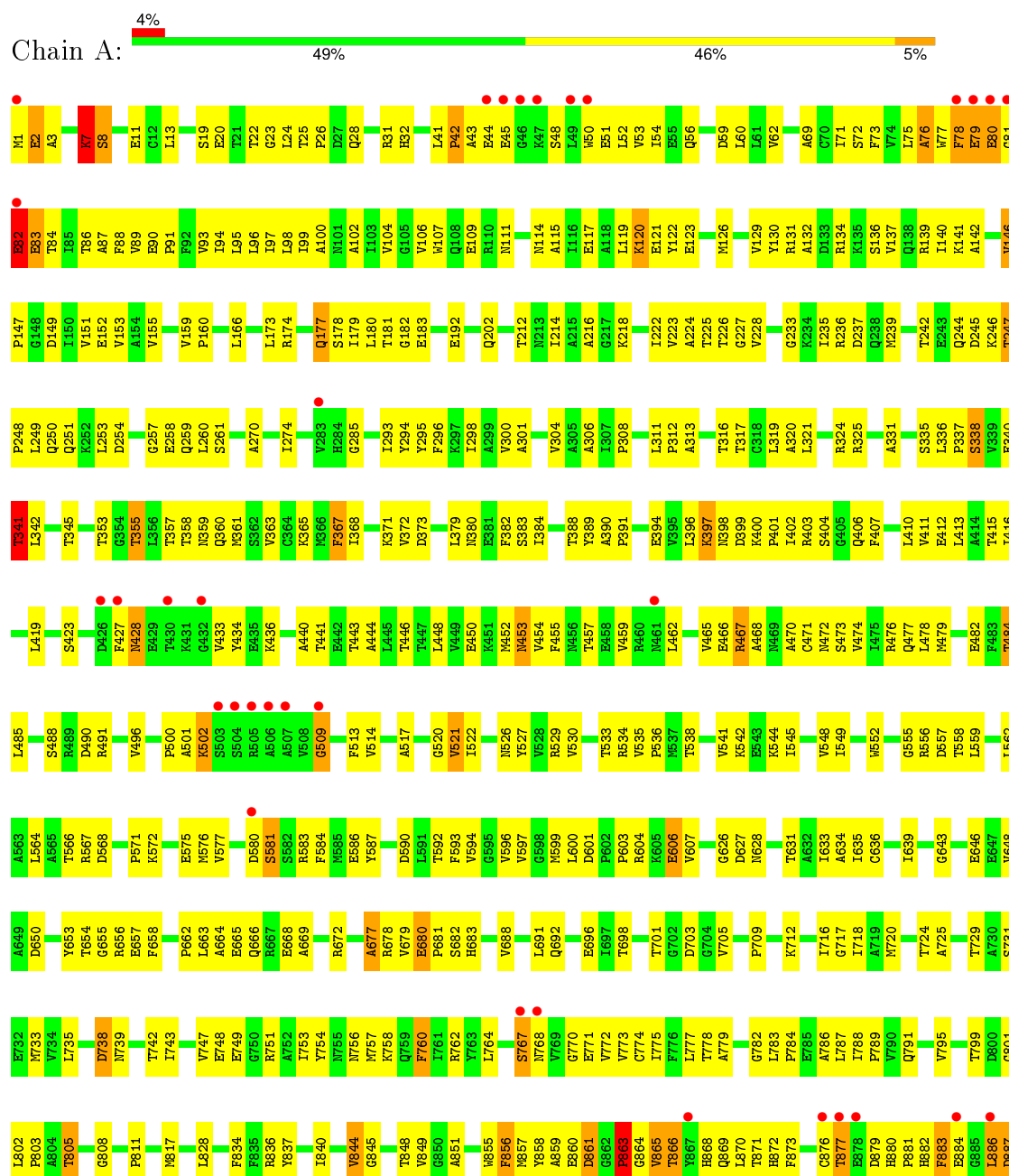
- Molecule 6 is water.

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

### 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 errors 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 ( $\text{RSRZ} > 2$ ). 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: SERCA1a





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.55Å 71.55Å 591.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-3.10) 88.4 (29.85-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 3.11Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.280 0.241 , 0.242	Depositor DCC
$R_{free}$ test set	825 reflections (3.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	100.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 26089 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, OTK, PTY

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	0.50	0/7812	0.71	2/10592 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	7	LYS	CB-CA-C	-5.22	99.95	110.40
1	A	7	LYS	C-N-CA	-5.19	108.72	121.70

There are no chirality outliers.

There are no planarity outliers.

### 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	7671	0	7766	521	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	36	0	38	12	0
5	A	24	0	21	2	0
6	A	3	0	0	0	0
All	All	7736	0	7825	531	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 34.

All (531) 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:950:VAL:HG12	1:A:951:ASP:H	1.00	1.10
1:A:654:THR:HG22	1:A:657:GLU:HG3	1.40	1.03
1:A:371:LYS:HE2	1:A:373:ASP:HB2	1.42	1.02
1:A:863:PRO:HG2	1:A:890:ILE:HG21	1.41	1.01
1:A:668:GLU:HG3	1:A:672:ARG:HH12	1.20	1.01
1:A:950:VAL:HG12	1:A:951:ASP:N	1.77	1.00
1:A:298:ILE:CD1	1:A:779:ALA:HB2	1.92	0.97
1:A:751:ARG:HD2	1:A:817:MET:HE2	1.47	0.96
1:A:950:VAL:CG1	1:A:951:ASP:H	1.79	0.94
1:A:680:GLU:HB2	1:A:681:PRO:HD2	1.49	0.92
1:A:865:VAL:HA	1:A:868:HIS:CE1	2.04	0.92
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.53	0.90
1:A:77:TRP:HD1	1:A:88:PHE:CZ	1.90	0.89
1:A:876:CYS:CB	1:A:888:CYS:SG	2.60	0.89
1:A:77:TRP:HD1	1:A:88:PHE:HZ	1.18	0.88
1:A:19:SER:OG	1:A:22:THR:HB	1.73	0.88
1:A:527:TYR:HB2	1:A:592:THR:HG22	1.57	0.87
1:A:248:PRO:HD2	1:A:341:THR:HG23	1.55	0.86
1:A:876:CYS:HB2	1:A:888:CYS:SG	2.15	0.86
1:A:77:TRP:CD1	1:A:88:PHE:HZ	1.94	0.86
1:A:397:LYS:HB2	1:A:402:ILE:CD1	2.06	0.86
1:A:788:ILE:HG23	1:A:789:PRO:HD2	1.57	0.85
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.57	0.85
1:A:331:ALA:HB1	1:A:733:MET:HE1	1.58	0.85
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.07	0.84
1:A:7:LYS:O	1:A:8:SER:HB3	1.76	0.84
1:A:312:PRO:O	1:A:316:THR:HG23	1.78	0.84
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.58	0.83
1:A:388:THR:HG22	1:A:389:TYR:H	1.44	0.83
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.61	0.83
1:A:1:MET:HA	1:A:224:ALA:O	1.79	0.83
1:A:247:THR:HG23	1:A:250:GLN:HG3	1.59	0.82
1:A:654:THR:HA	1:A:677:ALA:HB3	1.58	0.82
1:A:50:TRP:O	1:A:54:ILE:HG12	1.80	0.82
1:A:59:ASP:HB3	1:A:62:VAL:HG12	1.61	0.82
1:A:876:CYS:HB3	1:A:888:CYS:SG	2.19	0.82
1:A:81:GLY:O	1:A:82:GLU:HB3	1.77	0.82
1:A:342:LEU:O	1:A:345:THR:HG23	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:GLU:HB2	1:A:681:PRO:CD	2.10	0.81
1:A:453:ASN:HB3	1:A:471:CYS:SG	2.21	0.81
1:A:394:GLU:OE2	1:A:401:PRO:HB3	1.81	0.81
1:A:801:GLY:O	1:A:805:THR:HG23	1.81	0.80
1:A:909:MET:HE3	1:A:937:ILE:HG12	1.62	0.79
1:A:791:GLN:HB3	1:A:901:LEU:CD1	2.12	0.79
1:A:865:VAL:HG11	1:A:870:LEU:HB3	1.65	0.79
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.65	0.78
1:A:1:MET:HB2	1:A:225:THR:HG22	1.63	0.78
1:A:855:TRP:CE3	1:A:896:PRO:HG3	2.20	0.77
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.66	0.76
1:A:77:TRP:CE3	1:A:78:PHE:HB2	2.20	0.76
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.66	0.76
1:A:388:THR:HG22	1:A:389:TYR:N	1.99	0.75
1:A:662:PRO:HG2	1:A:665:GLU:OE1	1.86	0.75
1:A:247:THR:HG23	1:A:250:GLN:CG	2.16	0.75
1:A:545:ILE:O	1:A:549:ILE:HG12	1.87	0.74
1:A:126:MET:HG2	1:A:141:LYS:HA	1.69	0.74
1:A:654:THR:CG2	1:A:657:GLU:HG3	2.16	0.74
1:A:357:THR:HA	1:A:603:PRO:HA	1.70	0.74
1:A:411:VAL:HG22	1:A:454:VAL:CG1	2.19	0.73
1:A:865:VAL:O	1:A:865:VAL:HG12	1.88	0.73
1:A:397:LYS:HB2	1:A:402:ILE:HD11	1.71	0.73
1:A:530:VAL:O	1:A:530:VAL:HG23	1.87	0.73
1:A:836:ARG:O	1:A:840:ILE:HG12	1.89	0.73
1:A:311:LEU:HD13	1:A:764:LEU:HD12	1.70	0.72
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.68	0.72
1:A:397:LYS:HB2	1:A:402:ILE:HD12	1.71	0.72
1:A:775:ILE:O	1:A:778:THR:HG22	1.89	0.71
1:A:331:ALA:HB1	1:A:733:MET:CE	2.20	0.71
1:A:991:TYR:O	1:A:992:LEU:HB2	1.89	0.71
1:A:52:LEU:HD21	1:A:106:VAL:HA	1.73	0.71
1:A:82:GLU:HG3	1:A:83:GLU:N	2.04	0.70
1:A:239:MET:O	1:A:242:THR:HG22	1.91	0.70
1:A:102:ALA:O	1:A:106:VAL:HG12	1.91	0.70
1:A:411:VAL:HG22	1:A:454:VAL:HG11	1.72	0.70
1:A:558:THR:HG22	1:A:634:ALA:HB1	1.71	0.70
1:A:270:ALA:O	1:A:274:ILE:HG12	1.91	0.70
1:A:791:GLN:NE2	1:A:959:LEU:HD21	2.06	0.69
1:A:880:HIS:N	1:A:881:PRO:HD2	2.06	0.69
4:A:997:OTK:O11	4:A:997:OTK:O8	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:SER:HA	1:A:584:PHE:CD2	2.27	0.69
1:A:668:GLU:HG3	1:A:672:ARG:NH1	2.01	0.69
4:A:997:OTK:HO11	4:A:997:OTK:C27	2.05	0.69
1:A:894:PRO:O	1:A:898:THR:HG23	1.92	0.69
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.74	0.69
1:A:436:LYS:HG3	1:A:443:THR:HG21	1.75	0.69
1:A:869:GLN:HB3	1:A:872:HIS:ND1	2.07	0.69
1:A:298:ILE:HD13	1:A:779:ALA:HB2	1.74	0.68
1:A:751:ARG:HD2	1:A:817:MET:CE	2.23	0.68
1:A:606:GLU:CD	1:A:606:GLU:H	1.95	0.68
1:A:748:GLU:HA	1:A:817:MET:CE	2.23	0.68
1:A:879:ASP:C	1:A:881:PRO:HD2	2.14	0.68
1:A:648:VAL:O	1:A:648:VAL:HG12	1.93	0.68
1:A:131:ARG:NH1	1:A:149:ASP:OD2	2.26	0.68
1:A:988:ALA:HA	1:A:992:LEU:HD23	1.75	0.68
1:A:25:THR:HA	1:A:132:ALA:HB3	1.75	0.67
1:A:300:VAL:O	1:A:304:VAL:HG13	1.94	0.67
1:A:478:LEU:HD23	1:A:479:MET:HG2	1.76	0.67
1:A:7:LYS:O	1:A:8:SER:CB	2.40	0.67
1:A:22:THR:HG22	1:A:132:ALA:HB2	1.75	0.67
1:A:89:VAL:O	1:A:93:VAL:HG23	1.95	0.67
1:A:535:VAL:HG12	1:A:536:PRO:CD	2.25	0.66
1:A:836:ARG:HG2	1:A:984:LEU:HD13	1.75	0.66
1:A:192:GLU:OE1	1:A:580:ASP:HB2	1.95	0.66
1:A:969:MET:O	1:A:973:ILE:HG13	1.95	0.66
1:A:758:LYS:HG3	1:A:828:LEU:CD2	2.26	0.66
1:A:247:THR:HG23	1:A:250:GLN:CD	2.15	0.65
1:A:725:ALA:O	1:A:729:THR:HG23	1.96	0.65
1:A:471:CYS:O	1:A:474:VAL:HG22	1.96	0.65
1:A:898:THR:HG21	1:A:960:LYS:H	1.61	0.65
1:A:748:GLU:OE2	1:A:817:MET:HG3	1.96	0.65
1:A:79:GLU:O	1:A:80:GLU:HB2	1.97	0.65
1:A:863:PRO:HG2	1:A:890:ILE:CG2	2.24	0.64
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.78	0.64
1:A:472:ASN:O	1:A:476:ARG:HG3	1.97	0.64
1:A:688:VAL:O	1:A:692:GLN:HG3	1.98	0.64
1:A:87:ALA:O	1:A:88:PHE:HB2	1.98	0.64
1:A:535:VAL:HG12	1:A:536:PRO:HD2	1.80	0.64
1:A:173:LEU:HD12	1:A:216:ALA:O	1.98	0.64
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.80	0.63
1:A:32:HIS:CB	1:A:146:VAL:HG11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HG22	1:A:657:GLU:CG	2.24	0.63
1:A:757:MET:HA	1:A:760:PHE:CE2	2.33	0.63
1:A:748:GLU:HG3	1:A:817:MET:HE3	1.80	0.63
1:A:81:GLY:O	1:A:82:GLU:O	2.16	0.63
1:A:427:PHE:HB3	1:A:465:VAL:HA	1.80	0.63
1:A:691:LEU:O	1:A:696:GLU:HB2	1.98	0.63
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.29	0.63
1:A:549:ILE:HD11	1:A:596:VAL:HG11	1.80	0.63
1:A:909:MET:HE2	1:A:940:SER:HB2	1.82	0.62
1:A:60:LEU:HD21	1:A:261:SER:HB2	1.80	0.62
1:A:436:LYS:CG	1:A:443:THR:HG21	2.29	0.62
1:A:313:ALA:O	1:A:317:THR:HG23	2.00	0.62
1:A:748:GLU:HA	1:A:817:MET:HE3	1.82	0.61
1:A:788:ILE:HG23	1:A:789:PRO:CD	2.29	0.61
1:A:600:LEU:HD12	1:A:601:ASP:N	2.14	0.61
1:A:82:GLU:O	1:A:83:GLU:HB3	2.00	0.61
1:A:99:ILE:HG13	1:A:100:ALA:N	2.15	0.61
1:A:654:THR:HG23	1:A:656:ARG:H	1.66	0.61
1:A:183:GLU:OE2	1:A:202:GLN:HG3	2.00	0.61
1:A:857:MET:HG2	1:A:865:VAL:HB	1.80	0.61
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.30	0.61
1:A:249:LEU:HB2	1:A:340:GLU:OE1	2.00	0.61
1:A:25:THR:HB	1:A:26:PRO:HD2	1.82	0.61
1:A:1:MET:O	1:A:2:GLU:HB3	2.00	0.61
1:A:404:SER:OG	1:A:452:MET:HB2	2.00	0.61
1:A:69:ALA:HB2	1:A:94:ILE:HG21	1.83	0.61
1:A:865:VAL:HG22	1:A:868:HIS:NE2	2.16	0.60
1:A:95:LEU:O	1:A:99:ILE:HG12	2.00	0.60
1:A:654:THR:HG22	1:A:657:GLU:H	1.64	0.60
1:A:865:VAL:HG13	1:A:868:HIS:CD2	2.36	0.60
1:A:301:ALA:HB1	1:A:775:ILE:HD12	1.84	0.60
1:A:22:THR:HG22	1:A:132:ALA:CB	2.31	0.60
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.42	0.60
1:A:848:THR:HA	1:A:903:VAL:HG11	1.83	0.59
1:A:76:ALA:O	1:A:87:ALA:HB1	2.02	0.59
1:A:909:MET:CE	1:A:937:ILE:HA	2.33	0.59
1:A:407:PHE:O	1:A:411:VAL:HG23	2.01	0.59
1:A:90:GLU:OE2	1:A:789:PRO:HG2	2.01	0.59
1:A:114:ASN:HB3	1:A:117:GLU:HG2	1.84	0.59
1:A:500:PRO:HG3	1:A:509:GLY:HA2	1.84	0.59
1:A:73:PHE:HA	1:A:91:PRO:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:HB3	1:A:146:VAL:HG11	1.85	0.59
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.85	0.59
1:A:23:GLY:HA3	1:A:130:TYR:O	2.02	0.58
1:A:433:VAL:HG12	1:A:434:TYR:N	2.18	0.58
1:A:96:LEU:O	1:A:100:ALA:HB3	2.04	0.58
1:A:77:TRP:CD1	1:A:88:PHE:CZ	2.77	0.58
1:A:359:ASN:N	1:A:601:ASP:OD1	2.36	0.58
1:A:650:ASP:HB3	1:A:672:ARG:HE	1.69	0.58
1:A:388:THR:CG2	1:A:389:TYR:H	2.15	0.58
1:A:988:ALA:HA	1:A:992:LEU:CD2	2.34	0.57
1:A:179:ILE:HG13	1:A:180:LEU:N	2.19	0.57
1:A:398:ASN:O	1:A:399:ASP:HB2	2.03	0.57
1:A:32:HIS:HB3	1:A:146:VAL:CG1	2.35	0.57
1:A:358:THR:HG22	1:A:360:GLN:HB2	1.85	0.57
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.87	0.56
1:A:865:VAL:HA	1:A:868:HIS:HE1	1.64	0.56
1:A:462:LEU:HD13	1:A:466:GLU:OE1	2.05	0.56
1:A:179:ILE:O	1:A:705:VAL:HG12	2.05	0.56
1:A:863:PRO:CG	1:A:890:ILE:HG21	2.26	0.56
1:A:177:GLN:HB3	1:A:212:THR:HG21	1.88	0.56
1:A:419:LEU:HD12	1:A:513:PHE:CE2	2.40	0.56
1:A:907:ILE:HG23	1:A:977:VAL:HG21	1.87	0.56
1:A:367:PHE:CD2	1:A:596:VAL:HG22	2.41	0.56
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.41	0.56
1:A:703:ASP:O	1:A:724:THR:HG23	2.06	0.56
1:A:879:ASP:OD1	1:A:882:HIS:HB3	2.05	0.55
1:A:402:ILE:CG2	1:A:403:ARG:N	2.69	0.55
1:A:259:GLN:C	1:A:261:SER:H	2.10	0.55
1:A:791:GLN:HE21	1:A:959:LEU:HD21	1.71	0.55
1:A:861:ASP:O	1:A:861:ASP:CG	2.45	0.55
1:A:44:GLU:HG3	1:A:117:GLU:OE2	2.07	0.55
1:A:882:HIS:O	1:A:883:PHE:C	2.45	0.55
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.37	0.55
4:A:997:OTK:H1	4:A:997:OTK:O6	2.06	0.55
1:A:317:THR:O	1:A:321:LEU:HG	2.07	0.55
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.41	0.55
1:A:181:THR:OG1	1:A:183:GLU:HG3	2.07	0.55
1:A:249:LEU:CB	1:A:340:GLU:OE1	2.55	0.55
1:A:950:VAL:CG1	1:A:951:ASP:N	2.48	0.54
1:A:718:ILE:CG2	1:A:735:LEU:HG	2.37	0.54
1:A:382:PHE:CE2	1:A:410:LEU:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.38	0.54
1:A:367:PHE:C	1:A:367:PHE:CD1	2.81	0.54
1:A:680:GLU:CB	1:A:681:PRO:HD2	2.31	0.54
1:A:380:ASN:HB3	1:A:382:PHE:HE1	1.73	0.54
1:A:748:GLU:HA	1:A:817:MET:HE1	1.89	0.54
1:A:52:LEU:HD22	1:A:106:VAL:HB	1.90	0.54
1:A:855:TRP:CZ3	1:A:896:PRO:HG3	2.43	0.54
1:A:784:PRO:HG3	1:A:873:PHE:CD2	2.43	0.54
1:A:82:GLU:O	1:A:83:GLU:CB	2.56	0.53
1:A:126:MET:HA	1:A:142:ALA:H	1.71	0.53
1:A:488:SER:OG	1:A:491:ARG:NH1	2.42	0.53
1:A:450:GLU:OE1	1:A:467:ARG:NH1	2.41	0.53
1:A:107:TRP:CE2	1:A:111:ASN:ND2	2.76	0.53
1:A:119:LEU:O	1:A:121:GLU:N	2.41	0.53
1:A:398:ASN:C	1:A:400:LYS:H	2.12	0.53
1:A:701:THR:HB	1:A:720:MET:CE	2.39	0.53
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.91	0.53
1:A:391:PRO:HD2	1:A:434:TYR:CE2	2.44	0.53
1:A:383:SER:C	1:A:384:ILE:HD12	2.29	0.53
1:A:77:TRP:CZ3	1:A:78:PHE:HB2	2.44	0.53
1:A:248:PRO:O	1:A:251:GLN:HB2	2.09	0.53
1:A:228:VAL:HG13	1:A:237:ASP:OD2	2.09	0.53
1:A:59:ASP:HB3	1:A:62:VAL:CG1	2.34	0.53
1:A:60:LEU:HD21	1:A:261:SER:CB	2.38	0.53
1:A:717:GLY:O	1:A:731:SER:HB2	2.08	0.53
1:A:680:GLU:CB	1:A:681:PRO:CD	2.86	0.52
1:A:416:ILE:HG21	1:A:564:LEU:HB3	1.90	0.52
1:A:19:SER:HG	1:A:22:THR:HB	1.74	0.52
4:A:997:OTK:H4	4:A:997:OTK:H31B	1.90	0.52
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.39	0.52
1:A:767:SER:O	1:A:771:GLU:HG3	2.09	0.52
1:A:485:LEU:HD22	1:A:584:PHE:CE1	2.43	0.52
1:A:152:GLU:OE2	1:A:218:LYS:HE3	2.09	0.52
1:A:791:GLN:NE2	1:A:897:MET:HE2	2.24	0.52
1:A:898:THR:HG22	1:A:959:LEU:HA	1.91	0.52
1:A:791:GLN:HB3	1:A:901:LEU:HD11	1.89	0.52
1:A:88:PHE:C	1:A:91:PRO:HD2	2.30	0.52
1:A:566:THR:HG23	1:A:594:VAL:HG21	1.92	0.52
1:A:295:TYR:O	1:A:298:ILE:HG22	2.08	0.52
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.39	0.52
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:THR:HG22	1:A:634:ALA:CB	2.40	0.52
1:A:384:ILE:HD12	1:A:384:ILE:N	2.25	0.52
1:A:253:LEU:O	1:A:253:LEU:HD23	2.10	0.51
1:A:526:ASN:OD1	1:A:590:ASP:HA	2.10	0.51
1:A:192:GLU:CD	1:A:580:ASP:HB2	2.30	0.51
1:A:94:ILE:O	1:A:98:LEU:HG	2.10	0.51
1:A:361:MET:HB3	1:A:599:MET:HE3	1.90	0.51
1:A:626:GLY:O	1:A:678:ARG:HG2	2.10	0.51
1:A:501:ALA:O	1:A:502:LYS:HB2	2.11	0.51
1:A:254:ASP:O	1:A:258:GLU:HG2	2.11	0.51
1:A:631:THR:O	1:A:635:ILE:HG13	2.10	0.51
1:A:388:THR:HG22	1:A:390:ALA:H	1.76	0.51
1:A:541:VAL:O	1:A:545:ILE:HG13	2.11	0.51
1:A:79:GLU:O	1:A:80:GLU:CB	2.57	0.51
1:A:470:ALA:O	1:A:474:VAL:HG13	2.10	0.51
1:A:465:VAL:HG23	1:A:466:GLU:N	2.25	0.51
1:A:916:LEU:HD11	1:A:927:PRO:HA	1.91	0.51
1:A:749:GLU:O	1:A:753:ILE:HG12	2.10	0.51
1:A:777:LEU:HB2	1:A:849:VAL:HG21	1.92	0.51
1:A:236:ARG:O	1:A:236:ARG:HG2	2.10	0.51
1:A:840:ILE:O	1:A:844:VAL:HG13	2.11	0.50
1:A:83:GLU:HG3	1:A:84:THR:HG23	1.92	0.50
1:A:367:PHE:HA	1:A:380:ASN:O	2.10	0.50
1:A:758:LYS:O	1:A:762:ARG:HG3	2.11	0.50
1:A:783:LEU:HD12	1:A:871:THR:HG22	1.94	0.50
1:A:535:VAL:CG1	1:A:536:PRO:CD	2.90	0.50
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.93	0.50
1:A:7:LYS:HB3	1:A:11:GLU:HB2	1.93	0.50
1:A:581:SER:HA	1:A:584:PHE:CG	2.46	0.50
1:A:53:VAL:O	1:A:56:GLN:HB2	2.12	0.50
1:A:600:LEU:HD12	1:A:601:ASP:H	1.76	0.50
1:A:22:THR:CG2	1:A:132:ALA:CB	2.89	0.50
1:A:77:TRP:HE3	1:A:78:PHE:HB2	1.74	0.50
1:A:87:ALA:O	1:A:88:PHE:CB	2.60	0.50
1:A:248:PRO:CD	1:A:341:THR:HG23	2.35	0.50
1:A:60:LEU:CD2	1:A:261:SER:HB2	2.41	0.50
1:A:848:THR:HG22	1:A:903:VAL:HG13	1.92	0.50
1:A:325:ARG:HD2	1:A:749:GLU:OE1	2.12	0.50
1:A:298:ILE:HD11	1:A:779:ALA:HB2	1.87	0.49
1:A:126:MET:HB3	1:A:140:ILE:O	2.12	0.49
1:A:361:MET:HE3	1:A:599:MET:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:997:OTK:O10	4:A:997:OTK:H31	2.12	0.49
1:A:379:LEU:CD2	1:A:548:VAL:HG21	2.42	0.49
1:A:104:VAL:HG21	5:A:998:PTY:HC6	1.93	0.49
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.95	0.49
1:A:28:GLN:HG2	1:A:31:ARG:NH2	2.28	0.49
1:A:60:LEU:HD23	1:A:257:GLY:O	2.13	0.49
1:A:909:MET:CE	1:A:940:SER:HB2	2.42	0.49
4:A:997:OTK:O10	4:A:997:OTK:H9	2.12	0.49
1:A:583:ARG:HH11	1:A:583:ARG:HG2	1.78	0.49
1:A:45:GLU:HG3	1:A:45:GLU:O	2.12	0.49
1:A:654:THR:CG2	1:A:657:GLU:H	2.26	0.49
1:A:865:VAL:CG1	1:A:865:VAL:O	2.60	0.49
1:A:962:LEU:HD12	1:A:967:TRP:CD1	2.48	0.49
1:A:75:LEU:C	1:A:77:TRP:H	2.16	0.49
1:A:368:ILE:HD13	1:A:410:LEU:CD2	2.42	0.49
1:A:628:ASN:OD1	1:A:631:THR:HG23	2.13	0.49
1:A:48:SER:HB3	1:A:51:GLU:HG3	1.94	0.49
1:A:147:PRO:HG3	1:A:226:THR:HB	1.95	0.49
1:A:893:ALA:O	1:A:896:PRO:HD2	2.13	0.48
1:A:880:HIS:HA	1:A:884:GLU:HB2	1.95	0.48
1:A:782:GLY:O	1:A:873:PHE:HE2	1.96	0.48
1:A:441:THR:HB	1:A:599:MET:HE2	1.95	0.48
1:A:134:ARG:HH21	1:A:136:SER:HB2	1.78	0.48
1:A:758:LYS:HG3	1:A:828:LEU:HD22	1.95	0.48
1:A:455:PHE:HB2	1:A:457:THR:HG23	1.95	0.48
1:A:473:SER:O	1:A:477:GLN:HG3	2.14	0.48
1:A:772:VAL:HG21	4:A:997:OTK:H23	1.95	0.48
1:A:754:TYR:O	1:A:758:LYS:HB2	2.13	0.48
1:A:864:GLY:O	1:A:865:VAL:HG23	2.14	0.48
1:A:396:LEU:HD23	1:A:401:PRO:HA	1.95	0.48
1:A:126:MET:SD	1:A:139:ARG:NH1	2.87	0.48
1:A:402:ILE:HG22	1:A:403:ARG:N	2.29	0.48
1:A:335:SER:OG	1:A:338:SER:HB2	2.13	0.48
1:A:358:THR:O	1:A:359:ASN:HB3	2.13	0.48
1:A:898:THR:HG21	1:A:960:LYS:N	2.27	0.48
1:A:452:MET:O	1:A:454:VAL:N	2.47	0.48
1:A:865:VAL:HG21	1:A:870:LEU:HB3	1.95	0.47
1:A:249:LEU:HB2	1:A:340:GLU:CD	2.33	0.47
1:A:784:PRO:HG2	1:A:856:PHE:HE2	1.79	0.47
1:A:72:SER:OG	1:A:91:PRO:HG3	2.14	0.47
1:A:389:TYR:CE2	1:A:436:LYS:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASP:HB3	1:A:672:ARG:NE	2.30	0.47
1:A:992:LEU:HD12	1:A:993:GLU:OE1	2.14	0.47
1:A:413:LEU:HG	1:A:564:LEU:HD12	1.96	0.47
1:A:130:TYR:CE1	1:A:137:VAL:HB	2.49	0.47
1:A:433:VAL:CG1	1:A:434:TYR:N	2.76	0.47
1:A:52:LEU:CD2	1:A:106:VAL:HA	2.42	0.47
1:A:680:GLU:OE2	1:A:682:SER:HB3	2.14	0.47
1:A:568:ASP:OD2	1:A:592:THR:HG21	2.13	0.47
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.40	0.47
1:A:555:GLY:O	1:A:557:ASP:N	2.48	0.47
1:A:96:LEU:O	1:A:100:ALA:CB	2.62	0.47
1:A:811:PRO:HG2	1:A:929:VAL:HG13	1.96	0.47
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.96	0.47
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.77	0.47
1:A:235:ILE:HG23	1:A:709:PRO:HD3	1.95	0.47
1:A:756:ASN:ND2	1:A:808:GLY:O	2.42	0.47
1:A:79:GLU:HB3	1:A:293:ILE:HD11	1.97	0.47
1:A:527:TYR:O	1:A:592:THR:HA	2.14	0.47
1:A:368:ILE:HD13	1:A:410:LEU:HD23	1.96	0.47
1:A:865:VAL:HG13	1:A:868:HIS:CG	2.49	0.46
1:A:259:GLN:C	1:A:261:SER:N	2.68	0.46
1:A:42:PRO:HD3	1:A:228:VAL:HG23	1.96	0.46
1:A:535:VAL:HG12	1:A:536:PRO:N	2.30	0.46
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.96	0.46
1:A:980:LEU:O	1:A:984:LEU:HG	2.15	0.46
1:A:371:LYS:CE	1:A:373:ASP:HB2	2.31	0.46
1:A:86:THR:O	1:A:87:ALA:C	2.52	0.46
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.98	0.46
1:A:951:ASP:HB2	1:A:952:PRO:CD	2.38	0.46
1:A:662:PRO:O	1:A:664:ALA:N	2.49	0.46
1:A:758:LYS:HG3	1:A:828:LEU:HD21	1.95	0.46
1:A:391:PRO:HD2	1:A:434:TYR:CD2	2.50	0.46
1:A:791:GLN:HB3	1:A:901:LEU:HD12	1.94	0.46
1:A:876:CYS:SG	1:A:884:GLU:CD	2.94	0.46
1:A:93:VAL:O	1:A:97:ILE:HG12	2.16	0.46
1:A:919:ASN:O	1:A:989:ARG:HD3	2.15	0.46
1:A:941:MET:O	1:A:944:HIS:HB3	2.16	0.46
1:A:500:PRO:CG	1:A:509:GLY:HA2	2.46	0.46
1:A:735:LEU:HD11	1:A:743:ILE:CG1	2.46	0.46
1:A:444:ALA:HB3	1:A:599:MET:HE1	1.97	0.46
1:A:316:THR:HG21	5:A:998:PTY:HC52	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLU:O	1:A:468:ALA:N	2.49	0.46
1:A:903:VAL:O	1:A:907:ILE:HG13	2.15	0.46
1:A:865:VAL:O	1:A:866:THR:C	2.53	0.46
1:A:880:HIS:N	1:A:881:PRO:CD	2.76	0.46
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.97	0.45
1:A:109:GLU:OE1	1:A:109:GLU:C	2.54	0.45
1:A:978:ILE:O	1:A:982:GLU:HG2	2.15	0.45
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.69	0.45
1:A:436:LYS:HD2	1:A:440:ALA:HA	1.98	0.45
1:A:770:GLY:HA3	1:A:844:VAL:HG21	1.98	0.45
1:A:760:PHE:C	1:A:760:PHE:CD1	2.89	0.45
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.97	0.45
1:A:627:ASP:C	1:A:628:ASN:O	2.54	0.45
1:A:484:THR:HB	1:A:496:VAL:HG12	1.99	0.45
1:A:311:LEU:CD1	1:A:764:LEU:HD12	2.43	0.45
1:A:114:ASN:HB3	1:A:117:GLU:CG	2.46	0.45
1:A:178:SER:O	1:A:182:GLY:N	2.47	0.45
1:A:877:THR:HG23	1:A:888:CYS:CB	2.47	0.45
1:A:372:VAL:HG23	1:A:530:VAL:HG11	1.98	0.45
1:A:851:ALA:HB2	1:A:973:ILE:HD13	1.98	0.45
1:A:301:ALA:CB	1:A:775:ILE:HD12	2.47	0.45
1:A:837:TYR:HB2	4:A:997:OTK:H33	1.97	0.45
1:A:577:VAL:CG2	1:A:583:ARG:HE	2.29	0.45
1:A:397:LYS:CB	1:A:402:ILE:HD11	2.44	0.45
1:A:361:MET:HB3	1:A:599:MET:CE	2.46	0.45
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.17	0.45
1:A:71:ILE:O	1:A:75:LEU:HG	2.17	0.44
1:A:355:THR:HG21	1:A:720:MET:CE	2.47	0.44
1:A:517:ALA:O	1:A:521:VAL:HG13	2.18	0.44
1:A:534:ARG:CD	1:A:592:THR:HG21	2.47	0.44
1:A:246:LYS:O	1:A:247:THR:C	2.56	0.44
1:A:905:VAL:O	1:A:909:MET:HG2	2.17	0.44
1:A:648:VAL:O	1:A:648:VAL:CG1	2.63	0.44
1:A:747:VAL:O	1:A:747:VAL:HG12	2.17	0.44
1:A:900:ALA:HA	1:A:903:VAL:HG12	1.99	0.44
1:A:894:PRO:HD2	1:A:895:GLU:OE1	2.17	0.44
1:A:83:GLU:CG	1:A:84:THR:HG23	2.48	0.44
1:A:115:ALA:HB1	1:A:239:MET:HE1	1.99	0.44
1:A:99:ILE:CG1	1:A:100:ALA:N	2.80	0.44
1:A:41:LEU:HD21	1:A:233:GLY:HA2	2.00	0.44
1:A:653:TYR:CE2	1:A:669:ALA:HB1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HG23	1:A:656:ARG:N	2.30	0.44
1:A:72:SER:HB2	1:A:300:VAL:HG11	2.00	0.44
1:A:555:GLY:C	1:A:557:ASP:H	2.21	0.44
1:A:909:MET:CE	1:A:937:ILE:HG12	2.41	0.44
1:A:860:GLU:OE1	1:A:860:GLU:HA	2.17	0.44
1:A:81:GLY:O	1:A:82:GLU:CB	2.47	0.44
1:A:411:VAL:O	1:A:415:THR:HG23	2.18	0.44
1:A:567:ARG:NH1	1:A:571:PRO:HD3	2.33	0.44
1:A:865:VAL:HG13	1:A:868:HIS:CE1	2.52	0.44
1:A:121:GLU:O	1:A:121:GLU:CD	2.57	0.44
1:A:586:GLU:OE1	1:A:586:GLU:HA	2.18	0.44
1:A:895:GLU:N	1:A:896:PRO:CD	2.81	0.43
1:A:522:ILE:CG2	1:A:542:LYS:HE3	2.44	0.43
1:A:355:THR:HA	1:A:738:ASP:O	2.17	0.43
1:A:412:GLU:OE1	1:A:529:ARG:NE	2.51	0.43
1:A:527:TYR:CD2	1:A:592:THR:HG22	2.53	0.43
1:A:909:MET:HE1	1:A:937:ILE:HA	1.99	0.43
1:A:367:PHE:CE2	1:A:596:VAL:HG22	2.52	0.43
1:A:490:ASP:OD1	1:A:491:ARG:N	2.43	0.43
1:A:876:CYS:O	1:A:879:ASP:N	2.46	0.43
1:A:32:HIS:HB2	1:A:146:VAL:HG11	2.00	0.43
1:A:298:ILE:HD12	1:A:779:ALA:HB2	1.92	0.43
1:A:394:GLU:CD	1:A:401:PRO:HB3	2.39	0.43
1:A:909:MET:HE3	1:A:937:ILE:CG1	2.42	0.43
1:A:658:PHE:CZ	1:A:666:GLN:HG2	2.54	0.43
1:A:633:ILE:O	1:A:636:CYS:HB2	2.19	0.43
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.44	0.43
1:A:882:HIS:CD2	1:A:883:PHE:CD2	3.07	0.43
1:A:24:LEU:HG	1:A:149:ASP:HA	2.00	0.43
1:A:119:LEU:O	1:A:120:LYS:C	2.57	0.43
1:A:756:ASN:HB3	1:A:808:GLY:HA2	2.00	0.43
1:A:260:LEU:HG	1:A:260:LEU:O	2.18	0.43
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.82	0.43
1:A:900:ALA:O	1:A:903:VAL:HG12	2.18	0.43
1:A:679:VAL:HB	1:A:683:HIS:HB2	1.99	0.43
1:A:834:PHE:CD2	1:A:834:PHE:C	2.91	0.43
1:A:968:LEU:O	1:A:972:LYS:HG3	2.18	0.43
1:A:855:TRP:CA	1:A:859:ALA:HB2	2.48	0.43
1:A:898:THR:OG1	1:A:962:LEU:HD23	2.18	0.43
1:A:555:GLY:C	1:A:557:ASP:N	2.71	0.43
1:A:873:PHE:HB2	1:A:891:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:LEU:HD12	1:A:887:ASP:N	2.34	0.43
1:A:388:THR:CG2	1:A:389:TYR:N	2.69	0.43
4:A:997:OTK:C31	4:A:997:OTK:H4	2.48	0.43
1:A:301:ALA:HB1	1:A:775:ILE:CD1	2.48	0.43
1:A:882:HIS:CD2	1:A:883:PHE:HD2	2.37	0.43
1:A:178:SER:HB3	1:A:183:GLU:O	2.19	0.43
1:A:655:GLY:HA3	1:A:678:ARG:O	2.19	0.43
1:A:379:LEU:HD11	1:A:544:LYS:HG3	2.01	0.43
1:A:960:LYS:O	1:A:961:ALA:C	2.57	0.43
1:A:530:VAL:CG2	1:A:530:VAL:O	2.60	0.43
1:A:294:TYR:HD2	1:A:295:TYR:CD1	2.37	0.42
1:A:992:LEU:HG	1:A:993:GLU:H	1.83	0.42
1:A:964:LEU:O	1:A:964:LEU:HD23	2.19	0.42
1:A:73:PHE:HA	1:A:91:PRO:CG	2.48	0.42
1:A:606:GLU:CD	1:A:606:GLU:N	2.69	0.42
1:A:720:MET:HB3	1:A:738:ASP:OD1	2.20	0.42
1:A:576:MET:HE3	1:A:587:TYR:CD2	2.55	0.42
1:A:13:LEU:HD23	1:A:222:ILE:HD12	2.01	0.42
1:A:983:ILE:O	1:A:987:ILE:HG12	2.18	0.42
1:A:423:SER:O	1:A:446:THR:HG21	2.20	0.42
1:A:880:HIS:HA	1:A:884:GLU:CB	2.49	0.42
1:A:7:LYS:HB2	1:A:8:SER:H	1.56	0.42
1:A:1:MET:O	1:A:2:GLU:CB	2.64	0.42
1:A:382:PHE:CD1	1:A:382:PHE:N	2.87	0.42
1:A:877:THR:HG23	1:A:888:CYS:HB2	2.00	0.42
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.50	0.42
1:A:459:VAL:HG23	1:A:462:LEU:HD12	2.01	0.42
1:A:786:ALA:O	1:A:897:MET:HG2	2.19	0.42
1:A:76:ALA:HB1	1:A:88:PHE:H	1.84	0.42
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.84	0.42
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.54	0.42
1:A:20:GLU:HG3	1:A:166:LEU:HD13	2.01	0.42
1:A:778:THR:HG23	1:A:779:ALA:N	2.33	0.42
1:A:466:GLU:C	1:A:466:GLU:CD	2.78	0.42
1:A:635:ILE:O	1:A:639:ILE:HG12	2.20	0.42
1:A:379:LEU:N	1:A:379:LEU:HD12	2.35	0.42
1:A:778:THR:CG2	1:A:779:ALA:N	2.82	0.42
1:A:88:PHE:CA	1:A:91:PRO:HD2	2.50	0.42
1:A:534:ARG:HG3	1:A:535:VAL:N	2.35	0.41
1:A:411:VAL:CG2	1:A:454:VAL:HG11	2.47	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:997:OTK:C4	4:A:997:OTK:C31	2.98	0.41
1:A:363:VAL:HG21	1:A:448:LEU:HD22	2.03	0.41
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.83	0.41
1:A:78:PHE:CD2	1:A:79:GLU:CD	2.94	0.41
1:A:180:LEU:HG	1:A:180:LEU:O	2.21	0.41
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.87	0.41
1:A:828:LEU:HD23	1:A:828:LEU:HA	1.82	0.41
1:A:680:GLU:OE2	1:A:682:SER:CB	2.68	0.41
1:A:898:THR:HG22	1:A:959:LEU:CD2	2.51	0.41
1:A:840:ILE:HD13	1:A:980:LEU:HD23	2.02	0.41
1:A:857:MET:O	1:A:859:ALA:N	2.46	0.41
1:A:228:VAL:CG1	1:A:228:VAL:O	2.67	0.41
1:A:77:TRP:CE3	1:A:78:PHE:N	2.88	0.41
1:A:881:PRO:HG2	1:A:882:HIS:H	1.86	0.41
1:A:441:THR:HA	1:A:599:MET:CE	2.51	0.41
1:A:643:GLY:H	1:A:646:GLU:HB3	1.86	0.41
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.66	0.41
1:A:174:ARG:HB2	1:A:216:ALA:HB3	2.03	0.41
1:A:121:GLU:C	1:A:123:GLU:H	2.24	0.41
1:A:86:THR:HG22	1:A:86:THR:O	2.20	0.41
1:A:880:HIS:CE1	1:A:881:PRO:HD3	2.56	0.41
1:A:121:GLU:CD	1:A:121:GLU:C	2.80	0.41
1:A:577:VAL:HG23	1:A:583:ARG:HE	1.85	0.41
1:A:795:VAL:HA	1:A:799:THR:OG1	2.20	0.41
1:A:367:PHE:HZ	1:A:545:ILE:HG23	1.86	0.40
1:A:538:THR:OG1	1:A:541:VAL:HG23	2.21	0.40
1:A:244:GLN:OE1	1:A:712:LYS:HG2	2.21	0.40
1:A:840:ILE:HD13	1:A:980:LEU:CD2	2.50	0.40
1:A:320:ALA:O	1:A:324:ARG:HG3	2.21	0.40
1:A:864:GLY:O	1:A:865:VAL:CG2	2.70	0.40
1:A:898:THR:CG2	1:A:959:LEU:HA	2.51	0.40
1:A:81:GLY:C	1:A:82:GLU:O	2.60	0.40
1:A:603:PRO:O	1:A:604:ARG:C	2.59	0.40
1:A:119:LEU:C	1:A:121:GLU:N	2.73	0.40
1:A:681:PRO:O	1:A:682:SER:C	2.60	0.40
1:A:593:PHE:HZ	1:A:596:VAL:HG13	1.87	0.40
4:A:997:OTK:C1	4:A:997:OTK:O6	2.69	0.40
1:A:319:LEU:HD21	1:A:757:MET:CE	2.51	0.40
1:A:739:ASN:O	1:A:742:THR:HB	2.22	0.40
1:A:428:ASN:H	1:A:428:ASN:HD22	1.68	0.40
4:A:997:OTK:O3	4:A:997:OTK:H31A	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLU:C	1:A:468:ALA:N	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	992/994 (100%)	859 (87%)	87 (9%)	46 (5%)	<b>3</b> <b>17</b>

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	78	PHE
1	A	80	GLU
1	A	245	ASP
1	A	453	ASN
1	A	677	ALA
1	A	863	PRO
1	A	990	ASN
1	A	992	LEU
1	A	42	PRO
1	A	43	ALA
1	A	120	LYS
1	A	509	GLY
1	A	581	SER
1	A	663	LEU
1	A	738	ASP
1	A	865	VAL
1	A	886	LEU
1	A	950	VAL
1	A	2	GLU

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Mol	Chain	Res	Type
1	A	7	LYS
1	A	76	ALA
1	A	79	GLU
1	A	82	GLU
1	A	227	GLY
1	A	467	ARG
1	A	556	ARG
1	A	680	GLU
1	A	866	THR
1	A	961	ALA
1	A	3	ALA
1	A	122	TYR
1	A	353	THR
1	A	482	GLU
1	A	502	LYS
1	A	858	TYR
1	A	883	PHE
1	A	285	GLY
1	A	341	THR
1	A	397	LYS
1	A	951	ASP
1	A	974	SER
1	A	406	GLN
1	A	520	GLY
1	A	947	ILE
1	A	975	LEU

### 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	840/840 (100%)	811 (96%)	29 (4%)	43 78

All (29) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	82	GLU
1	A	83	GLU
1	A	146	VAL
1	A	177	GLN
1	A	247	THR
1	A	296	PHE
1	A	338	SER
1	A	341	THR
1	A	355	THR
1	A	367	PHE
1	A	428	ASN
1	A	484	THR
1	A	514	VAL
1	A	521	VAL
1	A	533	THR
1	A	597	VAL
1	A	606	GLU
1	A	698	THR
1	A	716	ILE
1	A	760	PHE
1	A	767	SER
1	A	805	THR
1	A	844	VAL
1	A	856	PHE
1	A	861	ASP
1	A	863	PRO
1	A	877	THR
1	A	887	ASP
1	A	890	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	868	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
4	OTK	A	997	-	36,38,38	0.86	1 (2%)	40,60,60	1.82	9 (22%)
5	PTY	A	998	-	22,23,49	1.79	2 (9%)	23,28,54	1.79	4 (17%)

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
4	OTK	A	997	-	-	0/22/84/84	0/3/3/3
5	PTY	A	998	-	-	0/27/27/53	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	997	OTK	O9-C10	-2.62	1.43	1.48
5	A	998	PTY	O4-C30	3.50	1.43	1.33
5	A	998	PTY	O30-C30	7.02	1.43	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	A	998	PTY	O4-C30-O30	-5.83	108.44	123.49
4	A	997	OTK	C6-O5-C12	-3.97	104.67	110.69
5	A	998	PTY	O30-C30-C31	-3.90	108.11	123.72
4	A	997	OTK	O12-C12-C11	-3.56	124.98	128.26
4	A	997	OTK	C3-O3-C21	-3.53	111.71	117.60
5	A	998	PTY	C6-O7-C8	-2.61	111.64	117.89
4	A	997	OTK	C2-C1-C5	-2.55	99.98	103.73
4	A	997	OTK	C26-C4-C3	-2.30	110.62	114.73
4	A	997	OTK	O3-C21-O4	-2.08	119.15	123.30
5	A	998	PTY	O7-C8-C11	2.43	119.76	110.96
4	A	997	OTK	O7-C27-C28	3.29	118.67	111.53
4	A	997	OTK	O3-C21-C22	3.55	120.87	111.67
4	A	997	OTK	O9-C32-C33	3.84	119.02	110.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	997	OTK	12	0
5	A	998	PTY	2	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	994/994 (100%)	-0.01	36 (3%)	46 23	55, 92, 130, 161	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	ARG	5.1
1	A	994	GLY	4.8
1	A	506	ALA	4.5
1	A	877	THR	4.1
1	A	283	VAL	3.4
1	A	430	THR	3.4
1	A	504	SER	3.2
1	A	81	GLY	3.2
1	A	461	ASN	3.2
1	A	45	GLU	3.0
1	A	878	GLU	3.0
1	A	884	GLU	2.9
1	A	79	GLU	2.8
1	A	507	ALA	2.8
1	A	993	GLU	2.7
1	A	888	CYS	2.7
1	A	426	ASP	2.7
1	A	82	GLU	2.6
1	A	47	LYS	2.5
1	A	767	SER	2.5
1	A	503	SER	2.5
1	A	46	GLY	2.4
1	A	78	PHE	2.3
1	A	49	LEU	2.3
1	A	427	PHE	2.3
1	A	886	LEU	2.2
1	A	580	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	432	GLY	2.1
1	A	768	ASN	2.1
1	A	1	MET	2.1
1	A	509	GLY	2.1
1	A	867	TYR	2.1
1	A	876	CYS	2.1
1	A	50	TRP	2.1
1	A	44	GLU	2.1
1	A	80	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
4	OTK	A	997	36/36	0.86	0.42	2.68	136,143,146,147	0
5	PTY	A	998	24/50	0.83	0.26	1.39	113,123,130,132	0
2	NA	A	995	1/1	0.88	0.26	1.38	46,46,46,46	0
3	MG	A	996	1/1	0.77	0.57	-	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.