



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:06 AM GMT

PDB ID : 3O1I
Title : Crystal Structure of the TorS sensor domain - TorT complex in the absence of ligand
Authors : Moore, J.O.; Hendrickson, W.A.
Deposited on : 2010-07-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

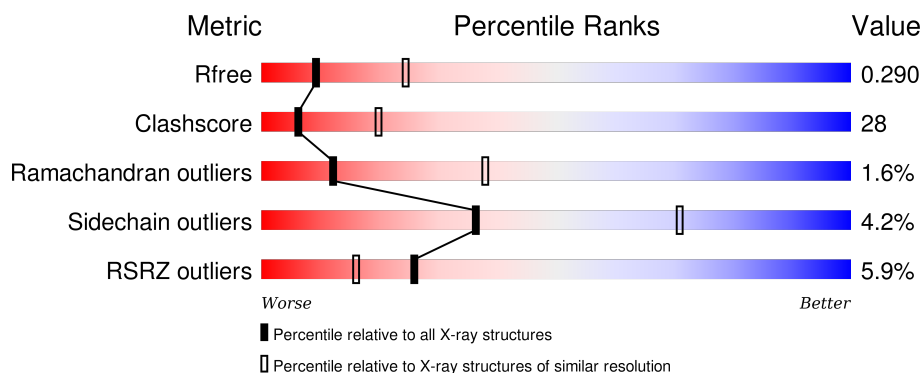
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	277	<div> <div>0%</div> <div>56%</div> <div>38%</div> <div>• •</div> </div>
1	B	277	<div> <div>4%</div> <div>58%</div> <div>36%</div> <div>• •</div> </div>
2	C	304	<div> <div>9%</div> <div>37%</div> <div>57%</div> <div>• •</div> </div>
2	D	304	<div> <div>8%</div> <div>51%</div> <div>43%</div> <div>• •</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9136 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 Sensor protein TorS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2162	1342	378	435	7			
1	B	270	Total	C	N	O	S	0	0	0
			2170	1346	380	437	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	EXPRESSION TAG	UNP Q87ID1
A	48	SER	-	EXPRESSION TAG	UNP Q87ID1
A	49	GLY	-	EXPRESSION TAG	UNP Q87ID1
A	50	SER	-	EXPRESSION TAG	UNP Q87ID1
A	323	LYS	PHE	CONFLICT	UNP Q87ID1
B	47	GLY	-	EXPRESSION TAG	UNP Q87ID1
B	48	SER	-	EXPRESSION TAG	UNP Q87ID1
B	49	GLY	-	EXPRESSION TAG	UNP Q87ID1
B	50	SER	-	EXPRESSION TAG	UNP Q87ID1
B	323	LYS	PHE	CONFLICT	UNP Q87ID1

- Molecule 2 is a protein called Periplasmic protein TorT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	295	Total	C	N	O	S	0	0	0
			2335	1482	402	444	7			
2	C	298	Total	C	N	O	S	0	0	0
			2350	1488	408	447	7			

There are 10 discrepancies between the modelled and reference sequences:

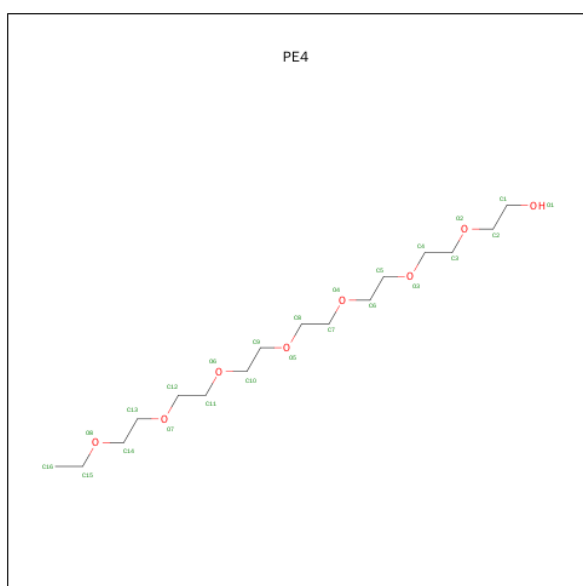
Chain	Residue	Modelled	Actual	Comment	Reference
D	26	GLY	-	EXPRESSION TAG	UNP Q87ID2
D	27	SER	-	EXPRESSION TAG	UNP Q87ID2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	28	GLY	-	EXPRESSION TAG	UNP Q87ID2
D	29	SER	-	EXPRESSION TAG	UNP Q87ID2
D	30	ASP	-	EXPRESSION TAG	UNP Q87ID2
C	26	GLY	-	EXPRESSION TAG	UNP Q87ID2
C	27	SER	-	EXPRESSION TAG	UNP Q87ID2
C	28	GLY	-	EXPRESSION TAG	UNP Q87ID2
C	29	SER	-	EXPRESSION TAG	UNP Q87ID2
C	30	ASP	-	EXPRESSION TAG	UNP Q87ID2

- Molecule 3 is 2-{2-[2-(2-{2-(2-ETHOXY-ETHOXY)-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			21	14	7		

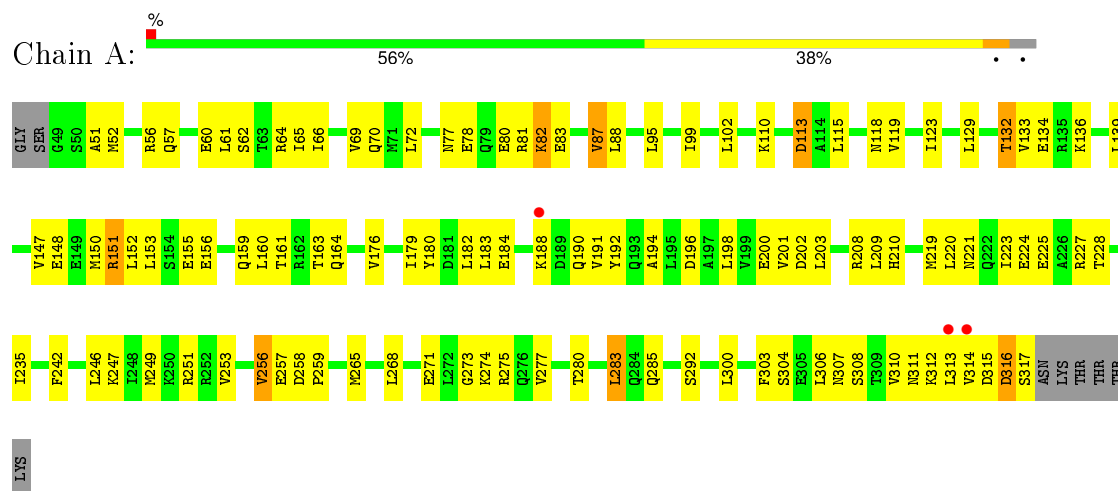
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	27	Total	O	0	0
			27	27		
4	D	17	Total	O	0	0
			17	17		
4	C	20	Total	O	0	0
			20	20		

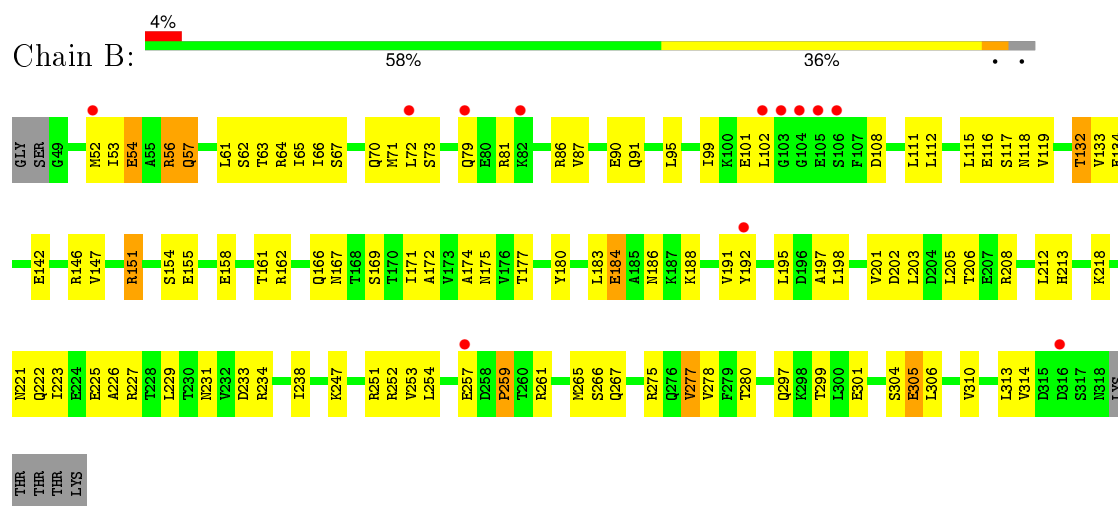
3 Residue-property plots

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 ($RSRZ > 2$). 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.

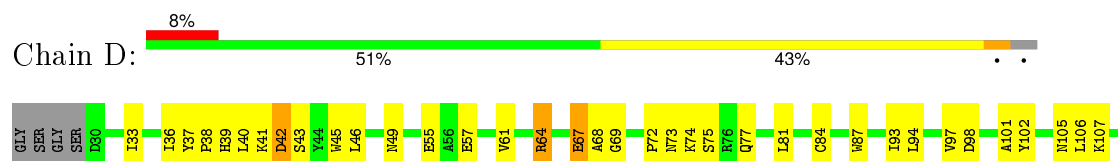
• Molecule 1: Sensor protein TorS

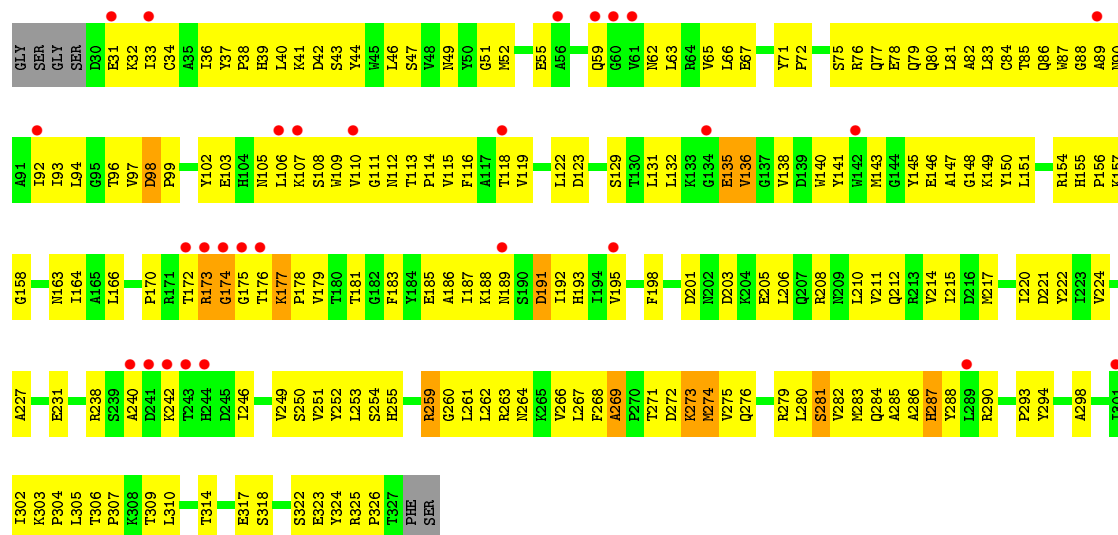


• Molecule 1: Sensor protein TorS



• Molecule 2: Periplasmic protein TorT





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.71Å 364.52Å 80.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.80 45.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-2.80) 99.8 (45.57-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.33 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.291 0.245 , 0.290	Depositor DCC
R_{free} test set	2107 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 42628 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9136	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: PE4

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	0.49	1/2177 (0.0%)	0.60	0/2936
1	B	0.45	1/2185 (0.0%)	0.57	0/2947
2	C	0.36	0/2404	0.64	0/3266
2	D	0.36	0/2389	0.61	0/3243
All	All	0.41	2/9155 (0.0%)	0.61	0/12392

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	GLU	CD-OE2	7.30	1.33	1.25
1	A	184	GLU	CD-OE2	6.96	1.33	1.25

There are no bond angle outliers.

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	2162	0	2201	105	0
1	B	2170	0	2207	116	0
2	C	2350	0	2316	195	1
2	D	2335	0	2296	125	1
3	B	21	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	34	0	0	4	0
4	B	27	0	0	2	0
4	C	20	0	0	5	0
4	D	17	0	0	2	0
All	All	9136	0	9044	504	2

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 28.

All (504) 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:256:VAL:HG12	1:A:257:GLU:H	1.18	1.08
2:C:224:VAL:HG12	2:C:249:VAL:HB	1.46	0.96
2:D:271:THR:HG22	2:D:273:LYS:H	1.33	0.93
2:C:166:LEU:HD23	2:C:224:VAL:HG23	1.51	0.91
2:C:93:ILE:HG22	2:C:118:THR:OG1	1.73	0.89
2:C:39:HIS:HD2	2:C:41:LYS:H	1.18	0.89
2:D:39:HIS:HD2	2:D:41:LYS:H	1.14	0.88
1:A:176:VAL:HG23	1:A:198:LEU:HD11	1.55	0.88
2:C:32:LYS:HB3	2:C:89:ALA:HA	1.57	0.87
2:C:59:GLN:HE22	2:C:283:MET:HA	1.45	0.82
1:A:256:VAL:HG12	1:A:257:GLU:N	1.94	0.81
2:C:85:THR:HG21	2:C:110:VAL:HA	1.63	0.81
2:C:43:SER:HB2	2:C:255:HIS:CD2	2.18	0.78
1:B:192:TYR:HE2	2:C:263:ARG:HH22	1.29	0.78
1:A:253:VAL:O	1:A:256:VAL:HG23	1.82	0.78
2:D:36:ILE:HD12	2:D:81:LEU:HD23	1.64	0.78
2:C:203:ASP:HB3	2:C:206:LEU:HG	1.66	0.77
2:C:44:TYR:CD1	2:C:274:MET:HG2	2.18	0.77
2:C:259:ARG:HH11	2:C:259:ARG:HB3	1.50	0.77
2:C:36:ILE:HD11	2:C:84:CYS:SG	2.25	0.76
1:B:54:GLU:HA	1:B:54:GLU:OE1	1.84	0.76
2:C:303:LYS:HD2	2:C:314:THR:HG21	1.69	0.75
2:D:106:LEU:HD21	2:D:115:VAL:HG11	1.69	0.75
2:D:271:THR:HG21	2:D:318:SER:OG	1.87	0.74
2:D:155:HIS:HB2	2:D:192:ILE:HD11	1.69	0.74
1:B:167:ASN:HD21	1:B:261:ARG:HH22	1.36	0.74
2:D:39:HIS:CD2	2:D:41:LYS:H	2.03	0.74
2:D:303:LYS:HG2	2:D:314:THR:HG21	1.70	0.74
2:C:106:LEU:HD21	2:C:115:VAL:HG11	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:OE1	1:A:268:LEU:HD21	1.88	0.74
2:D:214:VAL:HG13	2:D:220:ILE:HG13	1.70	0.73
2:D:46:LEU:HD13	2:D:326:PRO:HG3	1.70	0.73
1:B:306:LEU:O	1:B:310:VAL:HG13	1.89	0.73
1:B:158:GLU:OE2	1:B:213:HIS:HE1	1.71	0.72
1:A:151:ARG:HH11	1:A:151:ARG:HB3	1.54	0.72
1:B:167:ASN:HD22	1:B:261:ARG:HH12	1.38	0.71
1:A:219:MET:HG3	1:A:242:PHE:HE1	1.54	0.71
1:B:174:ALA:HB2	2:D:255:HIS:ND1	2.04	0.71
2:C:322:SER:C	2:C:324:TYR:H	1.94	0.71
2:C:44:TYR:HE2	2:C:173:ARG:HH22	1.37	0.71
1:A:219:MET:HG3	1:A:242:PHE:CE1	2.26	0.71
2:C:44:TYR:HD1	2:C:274:MET:HG2	1.55	0.70
1:A:192:TYR:CD1	1:B:183:LEU:HD23	2.26	0.70
1:A:235:ILE:HG21	1:A:283:LEU:HD13	1.72	0.70
2:C:90:ASN:O	2:C:114:PRO:HD2	1.90	0.70
2:C:146:GLU:OE1	2:C:304:PRO:HG3	1.90	0.70
2:D:49:ASN:HD21	2:D:327:THR:H	1.38	0.70
1:B:118:ASN:HD22	1:B:306:LEU:HA	1.58	0.69
2:C:276:GLN:HB2	2:C:317:GLU:HB3	1.75	0.69
2:C:55:GLU:HB2	2:C:279:ARG:HG2	1.72	0.69
2:D:107:LYS:HG2	2:D:131:LEU:HD11	1.75	0.69
2:D:143:MET:HE1	2:D:272:ASP:HB3	1.75	0.69
1:B:111:LEU:CD1	1:B:313:LEU:HD23	2.24	0.68
2:D:177:LYS:HB3	2:D:178:PRO:HD3	1.75	0.68
1:A:227:ARG:HG3	1:A:228:THR:HG23	1.76	0.68
2:C:32:LYS:H	2:C:90:ASN:ND2	1.92	0.68
1:A:151:ARG:HH12	1:A:152:LEU:HD23	1.57	0.68
2:D:224:VAL:HG22	2:D:249:VAL:HB	1.74	0.68
2:D:125:ASP:HB2	2:D:128:GLN:HG2	1.75	0.68
2:C:193:HIS:CE1	4:C:1:HOH:O	2.47	0.68
2:D:238:ARG:HG3	2:D:238:ARG:HH11	1.59	0.67
2:D:36:ILE:CD1	2:D:81:LEU:HD23	2.24	0.67
1:B:171:ILE:HD13	2:D:325:ARG:HG2	1.75	0.67
2:C:39:HIS:CD2	2:C:41:LYS:H	2.07	0.67
1:B:56:ARG:HG3	1:B:57:GLN:N	2.09	0.67
2:C:309:THR:O	2:C:309:THR:HG22	1.94	0.67
1:A:147:VAL:HG11	1:A:227:ARG:HB3	1.76	0.66
2:C:116:PHE:CZ	2:C:285:ALA:HA	2.31	0.66
1:B:95:LEU:O	1:B:99:ILE:HD13	1.95	0.66
1:B:253:VAL:HG21	1:B:265:MET:HB3	1.75	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:LYS:HB2	2:C:131:LEU:HD11	1.77	0.66
1:B:65:ILE:HD11	1:B:91:GLN:HB3	1.78	0.66
2:C:208:ARG:HB2	2:C:208:ARG:NH1	2.11	0.66
2:D:33:ILE:HD12	2:D:61:VAL:HG21	1.78	0.66
2:C:208:ARG:HH11	2:C:208:ARG:HB2	1.61	0.65
1:B:111:LEU:HB3	1:B:313:LEU:HD21	1.77	0.65
2:C:33:ILE:HG22	2:C:63:LEU:HD23	1.78	0.65
1:A:209:LEU:HD21	1:A:256:VAL:HG13	1.79	0.65
2:D:67:GLU:OE1	2:D:69:GLY:HA2	1.97	0.65
2:C:98:ASP:OD1	2:C:99:PRO:HD2	1.96	0.64
1:A:102:LEU:HG	1:A:313:LEU:HD22	1.80	0.64
1:B:102:LEU:HD21	1:B:310:VAL:HB	1.79	0.64
1:B:87:VAL:HG12	1:B:91:GLN:NE2	2.13	0.64
1:A:311:ASN:O	1:A:314:VAL:HG12	1.97	0.64
2:D:297:GLN:O	2:D:297:GLN:HG3	1.98	0.63
2:C:173:ARG:HD3	2:C:173:ARG:O	1.98	0.63
1:A:64:ARG:HD2	4:A:43:HOH:O	1.98	0.63
2:C:305:LEU:HD22	2:C:310:LEU:HD23	1.79	0.63
2:C:214:VAL:HA	2:C:217:MET:CE	2.27	0.63
2:D:164:ILE:HG22	2:D:222:TYR:HB2	1.79	0.63
2:D:125:ASP:H	2:D:128:GLN:HB2	1.62	0.63
2:C:105:ASN:O	2:C:108:SER:HB3	1.98	0.63
1:B:81:ARG:NH1	1:B:134:GLU:HG2	2.14	0.63
1:A:176:VAL:HG23	1:A:198:LEU:CD1	2.27	0.63
2:D:249:VAL:HG13	2:D:268:PHE:HB3	1.80	0.63
1:B:175:ASN:OD1	2:D:323:GLU:HG2	1.99	0.63
2:C:31:GLU:O	2:C:62:ASN:HB3	1.99	0.62
2:C:267:LEU:O	2:C:307:PRO:HD3	2.00	0.62
1:A:115:LEU:O	1:A:119:VAL:HG23	1.98	0.62
1:A:258:ASP:OD1	2:C:325:ARG:HD3	1.99	0.62
2:D:143:MET:CE	2:D:272:ASP:HB3	2.29	0.62
1:B:212:LEU:HD21	1:B:265:MET:CE	2.30	0.62
2:C:208:ARG:O	2:C:212:GLN:HG3	2.00	0.62
1:B:275:ARG:O	1:B:278:VAL:HG13	2.00	0.61
2:C:176:THR:HG22	2:C:177:LYS:H	1.65	0.61
1:B:111:LEU:HD12	1:B:313:LEU:HD23	1.83	0.61
1:B:197:ALA:HB2	2:C:238:ARG:NH2	2.16	0.61
1:B:192:TYR:CD2	2:C:263:ARG:NH2	2.69	0.61
1:A:198:LEU:O	1:A:203:LEU:HB2	2.01	0.61
1:B:86:ARG:O	1:B:90:GLU:HG3	2.00	0.61
2:D:93:ILE:HG22	2:D:118:THR:OG1	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:O	1:A:159:GLN:HG3	2.01	0.60
2:C:164:ILE:HG22	2:C:193:HIS:O	2.02	0.60
2:C:82:ALA:O	2:C:86:GLN:HG3	2.00	0.60
2:C:76:ARG:O	2:C:80:GLN:HG3	2.01	0.60
2:D:36:ILE:HD11	2:D:84:CYS:SG	2.41	0.60
1:B:167:ASN:ND2	1:B:261:ARG:HH22	1.99	0.60
1:B:61:LEU:HD23	1:B:64:ARG:HD3	1.83	0.60
1:A:102:LEU:O	1:A:313:LEU:HD21	2.02	0.60
2:C:136:VAL:HB	2:C:280:LEU:HG	1.82	0.60
2:D:42:ASP:HB3	2:D:45:TRP:H	1.67	0.59
2:C:32:LYS:HB2	2:C:90:ASN:ND2	2.16	0.59
2:D:106:LEU:O	2:D:110:VAL:HG22	2.03	0.59
2:C:176:THR:HG22	2:C:177:LYS:N	2.17	0.59
2:D:133:LYS:HE3	2:D:288:TYR:OH	2.02	0.59
1:B:192:TYR:HD2	2:C:263:ARG:CZ	2.16	0.59
2:C:253:LEU:HG	2:C:254:SER:N	2.18	0.59
1:A:192:TYR:CE2	2:D:263:ARG:NH2	2.70	0.59
2:D:261:LEU:HD11	2:D:269:ALA:HB3	1.85	0.58
2:C:179:VAL:HG11	2:C:251:VAL:HG11	1.84	0.58
2:D:204:LYS:HD2	2:D:232:ALA:HB2	1.85	0.58
2:C:322:SER:O	2:C:324:TYR:N	2.35	0.58
2:C:224:VAL:HG12	2:C:249:VAL:CB	2.27	0.58
1:A:271:GLU:HG3	1:A:275:ARG:NH1	2.18	0.58
1:B:247:LYS:HD2	4:B:333:HOH:O	2.04	0.58
2:C:288:TYR:HB2	2:C:294:TYR:CE2	2.38	0.58
1:A:200:GLU:OE2	2:D:265:LYS:HD2	2.03	0.58
2:D:112:ASN:HA	2:D:131:LEU:HD21	1.86	0.58
2:D:77:GLN:OE1	2:D:97:VAL:HG22	2.03	0.58
1:A:192:TYR:CE1	1:B:183:LEU:HD23	2.39	0.57
1:B:66:ILE:O	1:B:70:GLN:HG3	2.04	0.57
1:A:210:HIS:NE2	1:B:213:HIS:HD2	2.03	0.57
2:C:157:LYS:HD2	2:C:191:ASP:OD1	2.05	0.57
2:C:164:ILE:HD11	2:C:224:VAL:HG13	1.86	0.57
2:C:98:ASP:OD1	2:C:99:PRO:CD	2.52	0.57
2:C:268:PHE:CG	2:C:269:ALA:N	2.72	0.57
1:A:160:LEU:HD23	1:A:265:MET:HG2	1.86	0.57
2:C:85:THR:CG2	2:C:110:VAL:HA	2.33	0.57
2:D:43:SER:OG	2:D:255:HIS:CD2	2.58	0.57
2:D:151:LEU:HD11	2:D:224:VAL:HG21	1.87	0.57
1:B:301:GLU:O	1:B:304:SER:HB3	2.04	0.57
2:D:267:LEU:O	2:D:307:PRO:HD3	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:LYS:HB2	2:C:90:ASN:H	1.70	0.57
1:A:201:VAL:HG13	1:A:202:ASP:H	1.70	0.56
2:D:204:LYS:HG3	2:D:208:ARG:HH12	1.68	0.56
1:A:159:GLN:O	1:A:163:THR:HG23	2.04	0.56
1:A:208:ARG:HD3	2:D:208:ARG:NE	2.20	0.56
1:B:192:TYR:CE2	2:C:263:ARG:NH2	2.69	0.56
1:B:87:VAL:HG12	1:B:91:GLN:HE21	1.71	0.56
2:C:214:VAL:HA	2:C:217:MET:HE2	1.88	0.56
1:B:115:LEU:O	1:B:119:VAL:HG23	2.06	0.56
2:D:143:MET:HG3	2:D:251:VAL:O	2.06	0.56
1:A:182:LEU:HG	1:A:191:VAL:CG2	2.36	0.56
2:D:136:VAL:HG12	2:D:137:GLY:N	2.21	0.56
2:D:268:PHE:O	2:D:269:ALA:HB2	2.06	0.56
1:B:172:ALA:HA	1:B:202:ASP:OD1	2.06	0.56
2:C:85:THR:HG22	2:C:110:VAL:HG13	1.88	0.55
2:C:75:SER:O	2:C:79:GLN:HG2	2.06	0.55
1:B:166:GLN:OE1	2:D:41:LYS:HB3	2.06	0.55
1:A:182:LEU:HG	1:A:191:VAL:HG22	1.88	0.55
2:D:107:LYS:HG2	2:D:131:LEU:CD1	2.37	0.55
2:C:271:THR:HG23	2:C:271:THR:O	2.06	0.55
2:D:268:PHE:HE2	2:D:270:PRO:HG3	1.71	0.55
2:C:147:ALA:HA	2:C:268:PHE:CE2	2.41	0.55
2:C:224:VAL:HA	2:C:249:VAL:O	2.06	0.55
2:C:211:VAL:O	2:C:214:VAL:HB	2.07	0.55
2:C:97:VAL:O	2:C:98:ASP:HB2	2.07	0.55
1:B:257:GLU:OE1	2:D:325:ARG:NH1	2.40	0.54
2:C:208:ARG:HH11	2:C:208:ARG:CB	2.20	0.54
2:D:136:VAL:HG12	2:D:137:GLY:H	1.71	0.54
2:C:148:GLY:HA2	2:C:187:ILE:HD11	1.89	0.54
1:A:315:ASP:C	1:A:317:SER:H	2.11	0.54
2:D:116:PHE:CZ	2:D:285:ALA:HA	2.42	0.54
2:C:280:LEU:HD21	2:C:298:ALA:CB	2.38	0.54
2:C:198:PHE:HB3	2:C:210:LEU:HD22	1.89	0.54
2:D:117:ALA:HB3	2:D:135:GLU:HB2	1.89	0.54
2:C:33:ILE:O	2:C:63:LEU:HA	2.08	0.54
1:A:188:LYS:HZ3	1:B:186:ASN:CG	2.11	0.54
1:B:234:ARG:CZ	1:B:238:ILE:HD11	2.38	0.54
1:A:225:GLU:CD	1:B:225:GLU:HG3	2.27	0.54
2:C:164:ILE:HG13	2:C:222:TYR:HB2	1.89	0.54
2:C:322:SER:C	2:C:324:TYR:N	2.60	0.54
2:C:324:TYR:CG	2:C:325:ARG:N	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:271:THR:HG22	2:C:303:LYS:O	2.07	0.53
2:C:52:MET:HA	2:C:282:VAL:CG2	2.38	0.53
2:D:151:LEU:HD21	2:D:249:VAL:HG21	1.90	0.53
1:A:60:GLU:O	1:A:64:ARG:HG3	2.08	0.53
1:A:78:GLU:HG3	1:A:82:LYS:NZ	2.23	0.53
1:A:161:THR:HG22	1:A:265:MET:HE1	1.89	0.53
2:C:287:HIS:HD2	2:C:293:PRO:O	1.92	0.53
1:B:253:VAL:HG21	1:B:265:MET:CB	2.38	0.53
1:B:177:THR:O	1:B:180:TYR:HB2	2.09	0.53
2:C:163:ASN:HB3	2:C:195:VAL:CG2	2.38	0.53
2:C:210:LEU:O	2:C:214:VAL:HG23	2.09	0.53
2:C:147:ALA:HA	2:C:268:PHE:HE2	1.73	0.53
2:D:46:LEU:CD1	2:D:326:PRO:HG3	2.38	0.53
2:D:40:LEU:HD11	2:D:46:LEU:HA	1.90	0.53
1:A:56:ARG:O	1:A:60:GLU:HG3	2.09	0.53
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.73	0.53
1:B:67:SER:O	1:B:71:MET:HG2	2.08	0.53
1:A:256:VAL:CG1	1:A:257:GLU:N	2.67	0.53
1:B:192:TYR:CD2	2:C:263:ARG:NH1	2.77	0.53
2:D:81:LEU:HD21	2:D:94:LEU:HD13	1.91	0.53
1:A:132:THR:CG2	1:A:292:SER:HB2	2.39	0.53
2:D:98:ASP:HB3	2:D:101:ALA:HB2	1.92	0.52
2:C:214:VAL:HA	2:C:217:MET:HE3	1.90	0.52
2:C:110:VAL:HG12	2:C:113:THR:HB	1.91	0.52
2:D:67:GLU:HG2	2:D:69:GLY:H	1.73	0.52
1:A:306:LEU:O	1:A:310:VAL:HG13	2.09	0.52
1:A:164:GLN:OE1	1:A:256:VAL:HG11	2.08	0.52
2:D:113:THR:O	2:D:131:LEU:HD22	2.10	0.52
2:C:93:ILE:HG21	2:C:281:SER:HB3	1.91	0.52
2:C:140:TRP:HZ3	2:C:252:TYR:HB3	1.75	0.52
2:C:52:MET:HA	2:C:282:VAL:HG21	1.92	0.52
2:C:271:THR:HG1	2:C:318:SER:HG	1.55	0.52
1:B:188:LYS:HG2	1:B:192:TYR:HE1	1.75	0.51
2:D:262:LEU:HD12	2:D:310:LEU:HD12	1.92	0.51
1:B:305:GLU:OE1	1:B:305:GLU:HA	2.11	0.51
2:C:34:CYS:HB3	2:C:92:ILE:HG22	1.92	0.51
1:A:180:TYR:HD1	2:C:262:LEU:HD23	1.75	0.51
1:A:66:ILE:HD13	1:A:300:LEU:HD23	1.92	0.51
1:B:147:VAL:HG11	1:B:227:ARG:HB2	1.93	0.51
2:C:77:GLN:O	2:C:81:LEU:HB2	2.09	0.51
1:B:65:ILE:CD1	1:B:91:GLN:HB3	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:THR:HG21	2:C:122:LEU:HD13	1.92	0.51
2:C:280:LEU:HD11	2:C:298:ALA:HB3	1.92	0.51
1:A:95:LEU:O	1:A:99:ILE:HG12	2.11	0.51
2:C:240:ALA:O	2:C:242:LYS:HG3	2.09	0.51
1:B:111:LEU:HD13	1:B:313:LEU:HD23	1.91	0.51
2:C:55:GLU:O	2:C:282:VAL:HG11	2.11	0.50
1:B:62:SER:O	1:B:66:ILE:HG12	2.11	0.50
2:D:148:GLY:HA3	2:D:186:ALA:HB3	1.93	0.50
2:C:39:HIS:HA	2:C:67:GLU:OE2	2.11	0.50
2:D:200:ALA:CB	2:D:210:LEU:HD11	2.40	0.50
1:A:176:VAL:HA	1:A:179:ILE:HG12	1.93	0.50
2:D:203:ASP:HB3	2:D:206:LEU:HB2	1.93	0.50
1:B:108:ASP:O	1:B:112:LEU:HG	2.12	0.50
1:A:220:LEU:O	1:A:224:GLU:HG3	2.11	0.50
2:C:303:LYS:HD2	2:C:314:THR:CG2	2.41	0.50
1:B:118:ASN:ND2	1:B:306:LEU:HA	2.26	0.50
1:B:56:ARG:HG3	1:B:57:GLN:H	1.75	0.50
1:A:201:VAL:HG13	1:A:202:ASP:N	2.27	0.50
1:A:72:LEU:HG	1:A:133:VAL:HG21	1.94	0.50
1:B:191:VAL:O	1:B:195:LEU:HG	2.12	0.50
2:C:36:ILE:HG22	2:C:77:GLN:HE21	1.76	0.50
2:C:106:LEU:HD21	2:C:115:VAL:CG1	2.39	0.50
1:B:65:ILE:HD11	1:B:91:GLN:CB	2.40	0.50
1:A:57:GLN:HA	1:A:60:GLU:OE1	2.12	0.50
1:B:201:VAL:HG12	1:B:202:ASP:OD2	2.12	0.50
2:C:143:MET:SD	2:C:272:ASP:HB3	2.52	0.50
2:C:65:VAL:HG23	4:C:342:HOH:O	2.11	0.50
2:C:259:ARG:NH1	2:C:259:ARG:HB3	2.25	0.49
2:C:280:LEU:O	2:C:284:GLN:HG3	2.12	0.49
2:C:164:ILE:HD11	2:C:224:VAL:CG1	2.42	0.49
2:D:117:ALA:HB3	2:D:135:GLU:CB	2.42	0.49
2:D:145:TYR:CD1	2:D:186:ALA:HB2	2.47	0.49
2:C:141:TYR:OH	2:C:185:GLU:HG3	2.11	0.49
2:C:110:VAL:HG12	2:C:113:THR:CB	2.42	0.49
2:D:64:ARG:HB2	2:D:87:TRP:CH2	2.47	0.49
1:B:99:ILE:HG23	1:B:115:LEU:HD21	1.93	0.49
1:A:51:ALA:CB	1:A:314:VAL:HG23	2.42	0.49
2:C:195:VAL:HG21	2:C:220:ILE:HD13	1.94	0.49
1:A:164:GLN:NE2	1:A:265:MET:SD	2.85	0.49
1:B:197:ALA:HB2	2:C:238:ARG:HH21	1.75	0.49
2:D:220:ILE:N	4:D:339:HOH:O	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:268:PHE:O	2:C:269:ALA:HB2	2.12	0.48
1:A:132:THR:HG21	1:A:292:SER:HB2	1.94	0.48
2:C:148:GLY:HA3	2:C:187:ILE:HG12	1.95	0.48
2:C:260:GLY:HA3	2:C:266:VAL:HG23	1.94	0.48
1:B:177:THR:OG1	2:D:259:ARG:HG3	2.14	0.48
1:B:192:TYR:CD2	2:C:263:ARG:CZ	2.95	0.48
2:C:155:HIS:N	2:C:156:PRO:HD3	2.28	0.48
2:C:110:VAL:CG1	2:C:113:THR:HB	2.44	0.48
1:A:196:ASP:OD1	2:D:263:ARG:HG3	2.14	0.48
1:A:225:GLU:OE2	1:B:225:GLU:HG3	2.13	0.48
2:C:183:PHE:CZ	2:C:187:ILE:HG13	2.48	0.48
2:C:150:TYR:CD2	2:C:150:TYR:C	2.87	0.48
1:B:253:VAL:HG13	1:B:254:LEU:N	2.29	0.48
2:C:119:VAL:HG12	2:C:119:VAL:O	2.13	0.48
1:B:166:GLN:O	1:B:169:SER:HB3	2.14	0.48
2:C:286:ALA:O	2:C:290:ARG:HG3	2.14	0.48
2:C:146:GLU:CD	2:C:304:PRO:HG3	2.35	0.47
2:C:280:LEU:HD21	2:C:298:ALA:HB1	1.96	0.47
1:B:53:ILE:HA	1:B:56:ARG:HG2	1.96	0.47
2:D:230:ILE:HG13	2:D:250:SER:HB2	1.95	0.47
1:B:95:LEU:HG	1:B:99:ILE:HD13	1.96	0.47
1:A:253:VAL:HG21	1:A:265:MET:HB3	1.97	0.47
2:C:214:VAL:HG13	2:C:220:ILE:HG13	1.94	0.47
2:D:151:LEU:HD11	2:D:224:VAL:CG2	2.44	0.47
1:A:315:ASP:O	1:A:317:SER:N	2.48	0.47
1:B:162:ARG:HG2	1:B:166:GLN:NE2	2.29	0.47
2:D:155:HIS:HE2	2:D:222:TYR:HE1	1.61	0.47
2:C:158:GLY:H	2:C:191:ASP:CG	2.17	0.47
1:A:315:ASP:C	1:A:317:SER:N	2.68	0.47
2:C:145:TYR:CD1	2:C:186:ALA:HB2	2.50	0.47
1:B:226:ALA:HA	1:B:229:LEU:HD12	1.96	0.47
2:D:72:PRO:O	2:D:74:LYS:N	2.38	0.47
2:C:193:HIS:NE2	4:C:1:HOH:O	2.36	0.47
1:A:235:ILE:CG2	1:A:283:LEU:HD13	2.43	0.47
1:B:66:ILE:HD13	1:B:299:THR:HG22	1.96	0.47
1:B:184:GLU:C	1:B:186:ASN:H	2.17	0.47
2:D:238:ARG:NH1	2:D:238:ARG:HG3	2.27	0.47
2:C:32:LYS:HG3	2:C:88:GLY:O	2.14	0.46
2:C:42:ASP:HB3	2:C:44:TYR:H	1.81	0.46
2:C:181:THR:O	2:C:185:GLU:HG2	2.15	0.46
1:A:65:ILE:HG21	1:A:303:PHE:HZ	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:ALA:HB3	2:D:210:LEU:HD11	1.97	0.46
1:A:153:LEU:HD13	1:A:271:GLU:HB3	1.97	0.46
1:A:132:THR:HG21	1:A:292:SER:CB	2.45	0.46
1:A:70:GLN:OE1	1:B:297:GLN:HG3	2.14	0.46
2:C:47:SER:C	2:C:49:ASN:N	2.67	0.46
2:D:55:GLU:HG2	2:D:279:ARG:O	2.15	0.46
2:D:196:ASP:OD1	2:D:197:SER:N	2.48	0.46
2:D:102:TYR:HA	2:D:105:ASN:OD1	2.14	0.46
1:A:176:VAL:HA	1:A:179:ILE:CG1	2.46	0.46
2:D:155:HIS:HB2	2:D:192:ILE:CD1	2.42	0.46
1:A:283:LEU:HA	1:A:283:LEU:HD12	1.80	0.46
1:B:212:LEU:HD21	1:B:265:MET:HE1	1.96	0.46
1:A:52:MET:CE	1:B:52:MET:HG2	2.45	0.46
2:D:155:HIS:O	2:D:190:SER:HB2	2.15	0.46
2:D:261:LEU:HD11	2:D:269:ALA:CB	2.45	0.46
1:A:118:ASN:HD22	1:A:306:LEU:HA	1.81	0.46
2:C:188:LYS:HG3	2:C:189:ASN:N	2.31	0.46
2:C:37:TYR:CD2	2:C:40:LEU:HD13	2.51	0.46
2:C:324:TYR:O	2:C:325:ARG:HG3	2.16	0.46
1:A:160:LEU:HD23	1:A:265:MET:CG	2.46	0.46
1:A:183:LEU:HD23	1:B:192:TYR:CE1	2.51	0.46
1:B:61:LEU:CD2	1:B:64:ARG:HD3	2.45	0.46
2:C:280:LEU:HD11	2:C:298:ALA:CB	2.45	0.46
1:A:251:ARG:NH2	4:A:10:HOH:O	2.44	0.46
2:C:36:ILE:HD12	2:C:66:LEU:HB2	1.98	0.46
1:B:171:ILE:CD1	2:D:325:ARG:HG2	2.44	0.46
2:D:264:ASN:OD1	2:D:307:PRO:HB3	2.16	0.46
2:D:255:HIS:CD2	2:D:319:LEU:HD22	2.51	0.46
2:C:103:GLU:HA	2:C:123:ASP:O	2.15	0.46
2:C:106:LEU:HG	2:C:131:LEU:HD13	1.98	0.46
2:D:217:MET:O	2:D:219:ASN:N	2.49	0.46
2:C:78:GLU:HB3	2:C:109:TRP:CZ3	2.51	0.46
2:D:275:VAL:HG23	2:D:318:SER:C	2.36	0.45
2:C:32:LYS:N	2:C:90:ASN:ND2	2.63	0.45
2:C:261:LEU:HD11	2:C:269:ALA:HB3	1.98	0.45
1:A:87:VAL:CG2	1:A:88:LEU:N	2.79	0.45
2:D:125:ASP:HB2	2:D:128:GLN:CG	2.44	0.45
1:B:212:LEU:HD21	1:B:265:MET:HE3	1.97	0.45
1:A:78:GLU:OE1	1:A:78:GLU:HA	2.16	0.45
1:B:192:TYR:HD2	2:C:263:ARG:NH2	2.13	0.45
1:B:111:LEU:HB3	1:B:313:LEU:CD2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:ARG:NH1	2:D:267:LEU:HD13	2.31	0.45
2:D:268:PHE:CE2	2:D:270:PRO:HG3	2.52	0.45
1:B:151:ARG:O	1:B:155:GLU:HB2	2.17	0.45
2:D:238:ARG:HD3	2:D:238:ARG:O	2.16	0.45
2:C:201:ASP:CG	4:C:337:HOH:O	2.55	0.45
1:B:310:VAL:O	1:B:314:VAL:HG23	2.16	0.45
2:C:251:VAL:HG12	2:C:251:VAL:O	2.16	0.45
1:B:188:LYS:O	1:B:192:TYR:HD1	1.99	0.45
1:A:274:LYS:HE2	4:A:333:HOH:O	2.16	0.45
1:B:72:LEU:HG	1:B:133:VAL:HG21	1.98	0.45
1:A:257:GLU:HG2	1:A:258:ASP:OD1	2.17	0.45
2:C:55:GLU:HG3	2:C:55:GLU:O	2.17	0.45
1:A:180:TYR:CD1	2:C:262:LEU:HD23	2.52	0.44
2:C:145:TYR:CE2	2:C:149:LYS:HD3	2.52	0.44
2:C:151:LEU:O	2:C:192:ILE:HD11	2.16	0.44
2:C:94:LEU:HD21	2:C:102:TYR:CD1	2.52	0.44
2:D:55:GLU:HB2	2:D:279:ARG:HG2	1.99	0.44
2:D:166:LEU:HD12	2:D:197:SER:OG	2.17	0.44
1:A:161:THR:HG22	1:A:265:MET:CE	2.47	0.44
2:C:90:ASN:O	2:C:113:THR:HG23	2.16	0.44
2:D:255:HIS:HD2	2:D:319:LEU:HD22	1.80	0.44
2:D:170:PRO:HG3	2:D:201:ASP:HA	1.99	0.44
2:C:173:ARG:O	2:C:175:GLY:N	2.51	0.44
1:A:151:ARG:HH12	1:A:152:LEU:CD2	2.28	0.44
2:C:55:GLU:OE1	2:C:55:GLU:HA	2.18	0.44
2:C:132:LEU:HD21	2:C:135:GLU:OE2	2.17	0.44
2:C:154:ARG:HD3	2:C:222:TYR:OH	2.18	0.44
1:B:277:VAL:O	1:B:280:THR:N	2.51	0.44
2:C:85:THR:O	2:C:88:GLY:N	2.43	0.44
1:B:73:SER:HA	1:B:133:VAL:HG22	2.00	0.44
1:A:179:ILE:HD13	1:A:194:ALA:HB1	1.98	0.44
1:B:53:ILE:O	1:B:57:GLN:HB2	2.17	0.44
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.30	0.44
2:C:303:LYS:HA	2:C:304:PRO:HD3	1.88	0.44
2:D:268:PHE:CG	2:D:269:ALA:N	2.85	0.44
2:C:94:LEU:HD11	2:C:96:THR:HG22	1.99	0.44
2:C:221:ASP:O	2:C:246:ILE:HA	2.17	0.44
1:A:308:SER:O	1:A:312:LYS:HG3	2.18	0.44
2:D:210:LEU:O	2:D:214:VAL:HG23	2.17	0.44
2:C:176:THR:CG2	2:C:177:LYS:H	2.25	0.44
2:D:154:ARG:HH12	2:D:267:LEU:HD13	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:VAL:CG1	2:C:302:ILE:HD11	2.48	0.43
2:D:183:PHE:O	2:D:187:ILE:HG12	2.18	0.43
1:B:192:TYR:HD2	2:C:263:ARG:NH1	2.14	0.43
1:A:51:ALA:HB1	1:A:314:VAL:HG23	2.01	0.43
1:B:259:PRO:HD2	4:B:324:HOH:O	2.17	0.43
2:D:192:ILE:HG22	2:D:192:ILE:O	2.19	0.43
2:C:306:THR:H	2:C:309:THR:HB	1.84	0.43
2:D:37:TYR:HB3	2:D:38:PRO:HD2	1.99	0.43
1:A:198:LEU:HA	1:A:202:ASP:CB	2.48	0.43
2:D:166:LEU:HB3	2:D:168:LEU:HG	2.01	0.43
2:D:38:PRO:CB	2:D:97:VAL:HG12	2.49	0.43
2:D:277:GLN:HA	2:D:280:LEU:HD12	2.00	0.43
1:A:52:MET:HE1	1:B:52:MET:HG2	1.99	0.43
1:A:221:ASN:HD22	1:B:221:ASN:HD22	1.66	0.43
2:D:271:THR:HG21	2:D:318:SER:CB	2.49	0.43
2:C:44:TYR:OH	2:C:140:TRP:HZ2	2.02	0.43
2:D:164:ILE:HD11	2:D:194:ILE:HG12	2.01	0.43
2:C:51:GLY:HA3	2:C:275:VAL:O	2.19	0.43
2:C:66:LEU:HD13	2:C:83:LEU:HD23	2.01	0.43
2:C:187:ILE:HG22	2:C:187:ILE:O	2.19	0.43
2:C:94:LEU:HG	2:C:96:THR:HG23	2.01	0.43
1:B:61:LEU:HA	1:B:61:LEU:HD23	1.82	0.42
2:C:215:ILE:HG23	2:C:242:LYS:HD2	2.00	0.42
1:B:208:ARG:HD2	2:C:205:GLU:OE2	2.18	0.42
1:B:231:ASN:OD1	1:B:233:ASP:HB2	2.19	0.42
2:C:92:ILE:CD1	2:C:110:VAL:HG11	2.49	0.42
1:B:205:LEU:O	1:B:206:THR:C	2.58	0.42
2:D:140:TRP:HB3	2:D:179:VAL:HG22	2.01	0.42
1:A:304:SER:HB3	1:B:63:THR:CG2	2.50	0.42
2:D:258:TYR:C	2:D:260:GLY:N	2.71	0.42
2:C:85:THR:CG2	2:C:110:VAL:HG13	2.49	0.42
1:B:102:LEU:CD2	1:B:310:VAL:HB	2.48	0.42
2:D:75:SER:HB3	4:D:17:HOH:O	2.20	0.42
2:D:254:SER:OG	2:D:257:VAL:HG23	2.18	0.42
1:A:77:ASN:ND2	1:A:80:GLU:HG3	2.34	0.42
2:D:115:VAL:HG12	2:D:131:LEU:HB3	2.01	0.42
2:C:129:SER:C	2:C:131:LEU:H	2.22	0.42
1:B:218:LYS:O	1:B:222:GLN:HG3	2.19	0.42
2:C:43:SER:HB2	2:C:255:HIS:HD2	1.76	0.42
2:C:75:SER:HB2	4:C:333:HOH:O	2.20	0.42
2:D:136:VAL:HG12	2:D:277:GLN:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:NH2	1:A:134:GLU:HG3	2.34	0.42
1:B:161:THR:HG22	1:B:265:MET:HE3	2.01	0.42
2:D:117:ALA:H	2:D:132:LEU:HD11	1.85	0.42
1:A:110:LYS:O	1:A:113:ASP:HB2	2.20	0.42
1:B:212:LEU:CD2	1:B:265:MET:HE3	2.49	0.42
1:A:307:ASN:O	1:A:310:VAL:HG22	2.19	0.42
2:D:287:HIS:HD2	2:D:293:PRO:O	2.02	0.42
2:C:40:LEU:HD21	2:C:326:PRO:HB2	2.01	0.42
2:C:116:PHE:CE1	2:C:285:ALA:HA	2.55	0.42
2:D:277:GLN:HE21	2:D:277:GLN:HB2	1.64	0.42
1:A:61:LEU:O	1:A:62:SER:C	2.57	0.41
2:C:62:ASN:ND2	2:C:87:TRP:CH2	2.88	0.41
1:A:78:GLU:HG3	1:A:82:LYS:HZ1	1.85	0.41
2:D:260:GLY:HA3	2:D:266:VAL:HG23	2.02	0.41
1:A:246:LEU:HD21	1:A:273:GLY:CA	2.50	0.41
2:C:174:GLY:HA2	2:C:178:PRO:HG2	2.01	0.41
2:D:221:ASP:O	2:D:222:TYR:HD2	2.03	0.41
1:B:253:VAL:CG1	1:B:254:LEU:N	2.84	0.41
1:B:142:GLU:O	1:B:146:ARG:HG3	2.20	0.41
2:C:44:TYR:CE1	2:C:274:MET:HG2	2.55	0.41
2:C:107:LYS:O	2:C:111:GLY:N	2.46	0.41
2:D:169:GLY:C	2:D:200:ALA:O	2.58	0.41
1:B:205:LEU:O	1:B:208:ARG:HB3	2.19	0.41
1:A:271:GLU:O	1:A:275:ARG:HD3	2.20	0.41
2:D:263:ARG:HD3	2:D:263:ARG:HA	1.79	0.41
1:B:61:LEU:O	1:B:65:ILE:HG12	2.20	0.41
1:B:66:ILE:CD1	1:B:299:THR:HG22	2.50	0.41
1:A:249:MET:O	1:A:253:VAL:HB	2.21	0.41
2:C:166:LEU:HD23	2:C:224:VAL:CG2	2.35	0.41
1:B:253:VAL:HG23	1:B:265:MET:HE1	2.02	0.41
2:C:227:ALA:O	2:C:231:GLU:HG3	2.21	0.41
1:A:247:LYS:NZ	4:A:25:HOH:O	2.47	0.41
2:C:79:GLN:O	2:C:83:LEU:N	2.52	0.41
1:B:57:GLN:HB2	1:B:57:GLN:HE21	1.61	0.41
1:A:119:VAL:O	1:A:123:ILE:HG12	2.20	0.41
2:C:37:TYR:HB3	2:C:38:PRO:HD2	2.02	0.41
1:A:83:GLU:O	1:A:87:VAL:HG13	2.21	0.41
2:C:71:TYR:N	2:C:72:PRO:CD	2.84	0.41
1:A:258:ASP:HA	1:A:259:PRO:HD3	1.94	0.41
2:D:107:LYS:HE3	2:D:127:GLU:O	2.21	0.41
2:D:118:THR:HG22	2:D:119:VAL:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:VAL:HA	2:C:298:ALA:O	2.21	0.41
1:B:54:GLU:OE2	1:B:101:GLU:OE2	2.39	0.41
2:C:97:VAL:O	2:C:98:ASP:CB	2.69	0.41
2:C:145:TYR:HE2	2:C:149:LYS:HD3	1.87	0.41
1:A:150:MET:HB3	1:A:223:ILE:HD13	2.03	0.41
2:C:224:VAL:O	2:C:224:VAL:HG23	2.21	0.40
2:C:107:LYS:HG3	2:C:111:GLY:O	2.21	0.40
1:B:154:SER:HB2	1:B:223:ILE:HD12	2.03	0.40
1:A:139:LEU:HD13	1:A:285:GLN:HA	2.02	0.40
1:A:69:VAL:HB	1:A:129:LEU:CD2	2.51	0.40
2:D:271:THR:CG2	2:D:318:SER:OG	2.64	0.40
2:C:273:LYS:HB3	2:C:317:GLU:O	2.20	0.40
1:A:182:LEU:HD11	1:A:190:GLN:HB2	2.02	0.40
2:C:94:LEU:HD21	2:C:102:TYR:HD1	1.87	0.40
2:C:166:LEU:CD2	2:C:224:VAL:HG23	2.37	0.40
2:C:59:GLN:HE22	2:C:283:MET:CA	2.23	0.40
2:C:43:SER:HA	2:C:46:LEU:HB3	2.03	0.40
1:B:201:VAL:HG12	1:B:202:ASP:N	2.37	0.40
1:B:198:LEU:O	1:B:203:LEU:HG	2.21	0.40
1:B:251:ARG:HB2	1:B:251:ARG:HE	1.75	0.40
2:D:253:LEU:HD22	2:D:271:THR:OG1	2.21	0.40
1:B:132:THR:HG22	1:B:133:VAL:N	2.36	0.40
2:D:81:LEU:HD23	2:D:81:LEU:HA	1.92	0.40
1:A:61:LEU:O	1:A:64:ARG:N	2.50	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:LYS:NZ	2:D:161:LYS:NZ[3_654]	1.72	0.48
2:C:112:ASN:CB	2:C:112:ASN:CB[3_554]	2.03	0.17

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	267/277 (96%)	252 (94%)	13 (5%)	2 (1%)	26	62
1	B	268/277 (97%)	244 (91%)	23 (9%)	1 (0%)	39	74
2	C	296/304 (97%)	240 (81%)	46 (16%)	10 (3%)	5	16
2	D	291/304 (96%)	261 (90%)	25 (9%)	5 (2%)	11	36
All	All	1122/1162 (97%)	997 (89%)	107 (10%)	18 (2%)	12	38

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	73	ASN
2	D	170	PRO
2	C	170	PRO
2	C	273	LYS
2	D	68	ALA
2	D	269	ALA
2	C	173	ARG
2	C	174	GLY
1	A	316	ASP
2	C	264	ASN
2	C	323	GLU
1	A	256	VAL
1	B	259	PRO
2	C	98	ASP
2	C	172	THR
2	C	269	ALA
2	D	218	GLY
2	C	177	LYS

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/254 (97%)	236 (96%)	11 (4%)	34	68
1	B	248/254 (98%)	236 (95%)	12 (5%)	31	66
2	C	253/257 (98%)	245 (97%)	8 (3%)	46	80
2	D	252/257 (98%)	241 (96%)	11 (4%)	35	69
All	All	1000/1022 (98%)	958 (96%)	42 (4%)	36	71

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	87	VAL
1	A	113	ASP
1	A	132	THR
1	A	136	LYS
1	A	148	GLU
1	A	151	ARG
1	A	277	VAL
1	A	280	THR
1	A	283	LEU
1	A	316	ASP
1	B	54	GLU
1	B	56	ARG
1	B	57	GLN
1	B	79	GLN
1	B	116	GLU
1	B	117	SER
1	B	132	THR
1	B	151	ARG
1	B	266	SER
1	B	267	GLN
1	B	277	VAL
1	B	305	GLU
2	D	42	ASP
2	D	57	GLU
2	D	64	ARG
2	D	67	GLU
2	D	125	ASP
2	D	171	ARG
2	D	238	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	241	ASP
2	D	259	ARG
2	D	277	GLN
2	D	320	SER
2	C	135	GLU
2	C	136	VAL
2	C	191	ASP
2	C	250	SER
2	C	259	ARG
2	C	274	MET
2	C	281	SER
2	C	287	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	190	GLN
1	A	213	HIS
1	A	221	ASN
1	A	244	ASN
1	A	291	GLN
1	B	57	GLN
1	B	70	GLN
1	B	91	GLN
1	B	118	ASN
1	B	125	ASN
1	B	167	ASN
1	B	213	HIS
2	D	39	HIS
2	D	49	ASN
2	D	86	GLN
2	D	193	HIS
2	D	255	HIS
2	D	287	HIS
2	C	39	HIS
2	C	59	GLN
2	C	62	ASN
2	C	90	ASN
2	C	189	ASN
2	C	255	HIS
2	C	287	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	292	GLN
2	C	311	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PE4	B	1	-	20,20,23	0.93	0	19,19,22	0.52	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	PE4	B	1	-	-	0/18/18/21	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/277 (97%)	0.12	3 (1%) 82 74	19, 53, 89, 102	0
1	B	270/277 (97%)	0.17	12 (4%) 38 26	27, 55, 96, 110	0
2	C	298/304 (98%)	0.65	28 (9%) 11 5	38, 77, 102, 121	0
2	D	295/304 (97%)	0.43	24 (8%) 15 7	35, 67, 103, 109	0
All	All	1132/1162 (97%)	0.35	67 (5%) 26 16	19, 64, 100, 121	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	289	LEU	5.9
2	D	161	LYS	5.2
2	C	241	ASP	4.9
2	C	56	ALA	4.4
2	C	173	ARG	4.2
2	C	118	THR	4.1
2	C	134	GLY	4.1
2	D	184	TYR	3.9
2	D	162	THR	3.9
2	D	192	ILE	3.9
2	C	172	THR	3.9
2	C	175	GLY	3.4
2	C	174	GLY	3.2
1	B	104	GLY	3.1
2	D	160	GLY	3.1
1	B	79	GLN	3.0
2	C	60	GLY	3.0
2	D	191	ASP	3.0
2	C	89	ALA	2.9
2	D	194	ILE	2.9
2	D	187	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	189	ASN	2.8
2	D	153	GLU	2.8
2	D	193	HIS	2.7
2	D	126	GLU	2.7
2	C	110	VAL	2.7
2	D	219	ASN	2.7
2	C	189	ASN	2.7
2	D	157	LYS	2.7
1	A	314	VAL	2.6
2	D	242	LYS	2.6
1	B	105	GLU	2.6
2	C	301	ILE	2.6
1	A	313	LEU	2.6
1	B	106	SER	2.6
2	D	220	ILE	2.6
2	D	124	LEU	2.5
2	D	156	PRO	2.5
2	C	195	VAL	2.5
1	B	103	GLY	2.4
2	D	159	SER	2.4
1	B	102	LEU	2.4
2	C	176	THR	2.4
2	C	31	GLU	2.4
2	C	59	GLN	2.4
2	D	199	TRP	2.4
2	C	244	HIS	2.4
2	C	33	ILE	2.3
2	C	240	ALA	2.3
2	C	92	ILE	2.3
1	B	192	TYR	2.3
2	D	244	HIS	2.2
1	B	257	GLU	2.2
2	C	106	LEU	2.2
1	B	316	ASP	2.2
2	C	61	VAL	2.2
2	D	293	PRO	2.2
2	D	185	GLU	2.2
2	C	107	LYS	2.2
2	C	242	LYS	2.2
1	A	188	LYS	2.2
2	C	243	THR	2.1
1	B	72	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	LYS	2.1
2	C	142	TRP	2.1
1	B	52	MET	2.0
2	D	190	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PE4	B	1	21/24	0.87	0.22	1.28	58,61,72,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.