Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:04 AM GMT

PDB ID	:	3H2U
Title	:	Human raver1 RRM1, RRM2, and RRM3 domains in complex with human vinculin tail domain Vt
Authors	:	Lee, J.H.; Rangarajan, E.S.; Yogesha, S.D.; Izard, T.
Deposited on	:	2009-04-14
Resolution	:	2.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

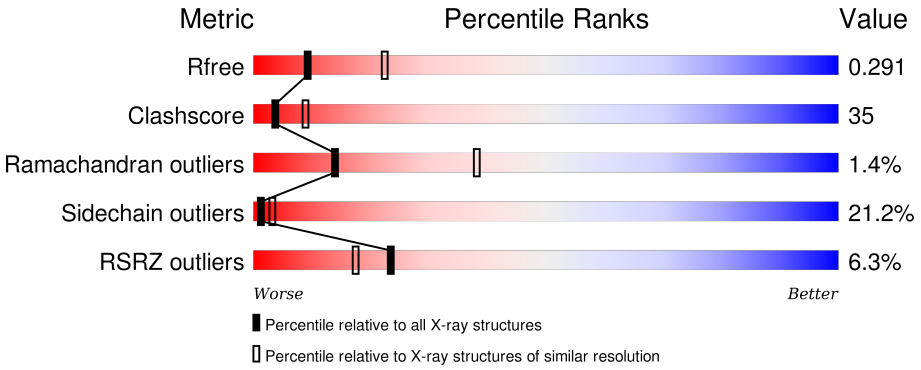
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 <=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	188	4% 55% 29% 11%
1	C	188	12% 42% 42% 9% 7%
2	B	283	3% 48% 38% 12%
2	D	283	7% 48% 38% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7167 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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1414	867	264	271	12			
1	C	174	Total	C	N	O	S	0	0	0
			1364	839	255	258	12			

- Molecule 2 is a protein called Raver-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2170	1361	389	408	12			
2	D	280	Total	C	N	O	S	0	0	0
			2178	1367	390	409	12			

- Molecule 3 is water.

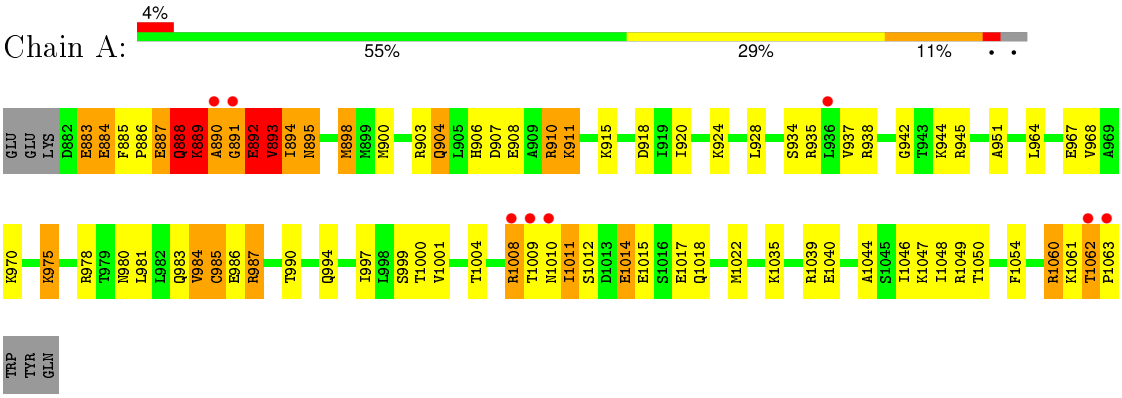
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	15	Total	O	0	0
			15	15		
3	C	3	Total	O	0	0
			3	3		
3	D	9	Total	O	0	0
			9	9		

3 Residue-property plots (i)

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.

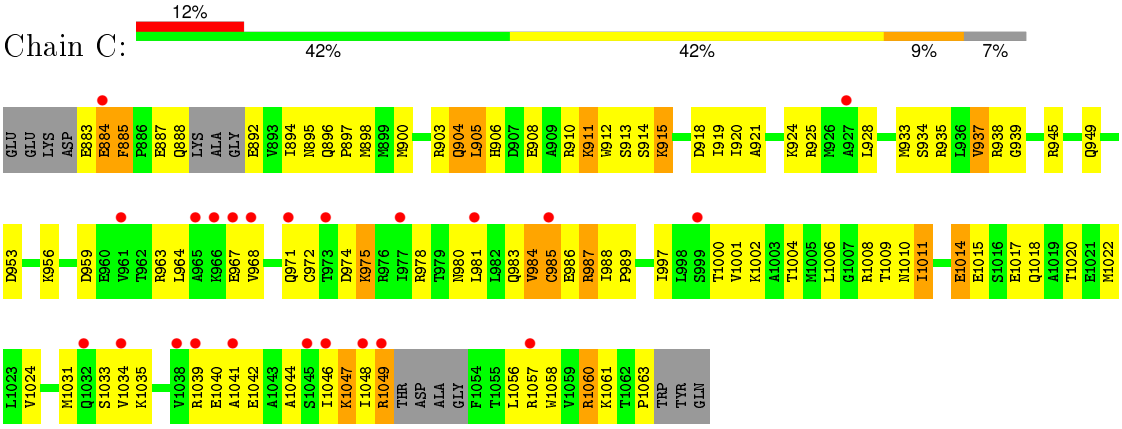
- Molecule 1: Vinculin

Chain A:



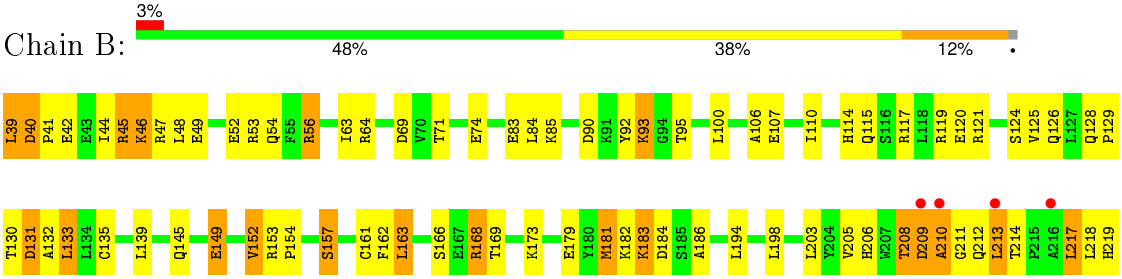
- Molecule 1: Vinculin

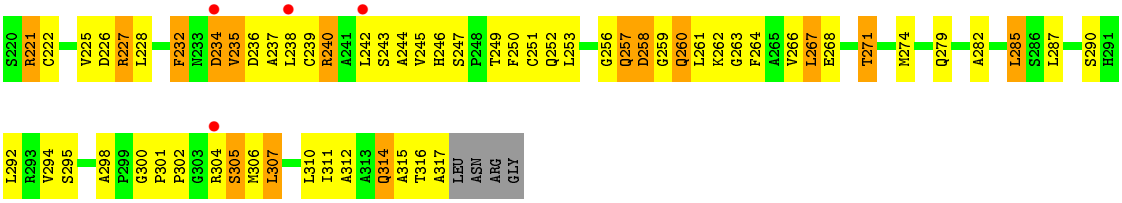
Chain C:



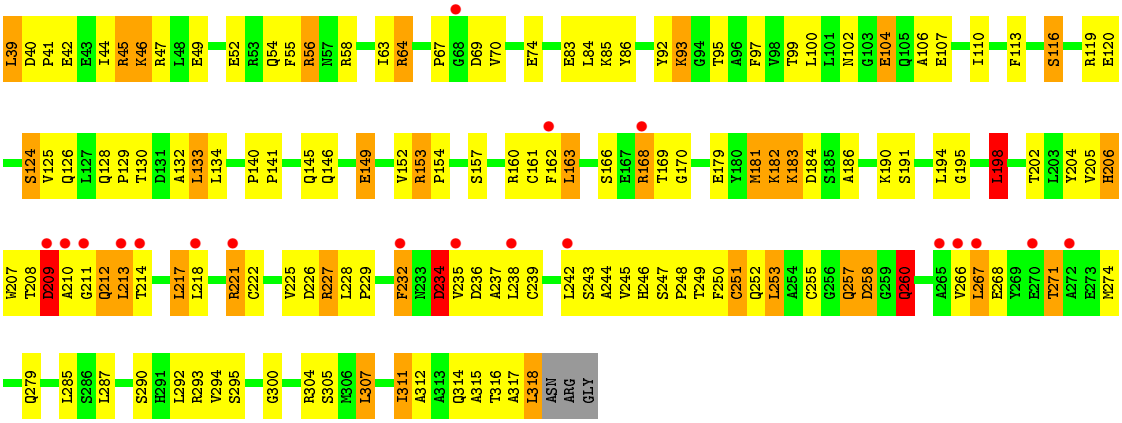
- Molecule 2: Raver-1

Chain B:





- Molecule 2: Raver-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.75Å 94.91Å 186.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 47.45 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.75) 99.8 (47.45-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 2.77Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.225 , 0.274 0.238 , 0.291	Depositor DCC
R_{free} test set	2024 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 40618 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7167	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.35	20/1425 (1.4%)	0.94	4/1911 (0.2%)
1	C	0.59	0/1373	0.72	0/1838
2	B	0.68	0/2213	0.84	2/2994 (0.1%)
2	D	0.60	0/2221	0.80	1/3005 (0.0%)
All	All	0.82	20/7232 (0.3%)	0.83	7/9748 (0.1%)

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
2	B	0	2
2	D	0	3
All	All	0	6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	892	GLU	CD-OE2	-15.37	1.08	1.25
1	A	893	VAL	CB-CG2	-14.41	1.22	1.52
1	A	893	VAL	CB-CG1	-12.96	1.25	1.52
1	A	892	GLU	CG-CD	-12.06	1.33	1.51
1	A	894	ILE	CA-CB	-10.69	1.30	1.54
1	A	894	ILE	CB-CG2	-10.21	1.21	1.52
1	A	892	GLU	CD-OE1	-9.87	1.14	1.25
1	A	893	VAL	CA-CB	-9.73	1.34	1.54
1	A	893	VAL	C-O	-8.71	1.06	1.23
1	A	894	ILE	C-O	-8.69	1.06	1.23
1	A	889	LYS	CB-CG	-8.07	1.30	1.52
1	A	892	GLU	C-O	-5.97	1.12	1.23
1	A	893	VAL	N-CA	-5.80	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	894	ILE	CB-CG1	-5.68	1.38	1.54
1	A	888	GLN	C-O	-5.67	1.12	1.23
1	A	894	ILE	N-CA	-5.67	1.35	1.46
1	A	889	LYS	CA-CB	-5.56	1.41	1.53
1	A	893	VAL	CA-C	-5.54	1.38	1.52
1	A	889	LYS	CD-CE	-5.53	1.37	1.51
1	A	890	ALA	CA-CB	-5.36	1.41	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	893	VAL	CG1-CB-CG2	-10.27	94.46	110.90
1	A	1062	THR	C-N-CD	-9.39	99.93	120.60
1	A	894	ILE	CG1-CB-CG2	-8.54	92.61	111.40
2	D	198	LEU	N-CA-C	-5.58	95.94	111.00
1	A	893	VAL	CB-CA-C	-5.22	101.48	111.40
2	B	152	VAL	CG1-CB-CG2	5.14	119.13	110.90
2	B	290	SER	N-CA-C	5.07	124.70	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	892	GLU	Peptide
2	B	208	THR	Peptide
2	B	210	ALA	Peptide
2	D	208	THR	Peptide
2	D	209	ASP	Peptide
2	D	234	ASP	Peptide

5.2 Too-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 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	1414	0	1469	88	0
1	C	1364	0	1423	92	0
2	B	2170	0	2147	169	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2178	0	2158	174	0
3	A	14	0	0	0	0
3	B	15	0	0	0	0
3	C	3	0	0	0	0
3	D	9	0	0	0	0
All	All	7167	0	7197	505	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 35.

All (505) 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)
2:D:234:ASP:O	2:D:253:LEU:HD11	1.42	1.16
1:A:891:GLY:HA3	1:A:892:GLU:CB	1.76	1.16
2:B:209:ASP:OD2	2:B:211:GLY:N	1.80	1.14
2:D:209:ASP:N	2:D:211:GLY:HA3	1.61	1.14
1:A:1062:THR:HB	1:A:1063:PRO:CD	1.77	1.14
1:A:888:GLN:O	1:A:889:LYS:HG2	1.48	1.12
2:B:258:ASP:HB2	2:B:260:GLN:HG2	1.24	1.11
1:A:891:GLY:CA	1:A:892:GLU:CB	2.28	1.10
2:B:235:VAL:HG22	2:B:253:LEU:HD13	1.32	1.10
2:B:235:VAL:HG13	2:B:253:LEU:HD12	1.35	1.09
2:D:130:THR:HB	2:D:210:ALA:HB2	1.35	1.09
2:B:209:ASP:N	2:B:210:ALA:HA	1.50	1.07
2:D:234:ASP:OD1	2:D:237:ALA:N	1.88	1.07
1:A:891:GLY:CA	1:A:892:GLU:HB2	1.78	1.07
2:D:232:PHE:CE1	2:D:287:LEU:HD21	1.90	1.06
1:A:1062:THR:CB	1:A:1063:PRO:HD2	1.88	1.03
1:A:1062:THR:HB	1:A:1063:PRO:HD2	1.38	1.02
1:C:1060:ARG:HG3	1:C:1060:ARG:HH11	1.20	1.02
2:D:209:ASP:CA	2:D:211:GLY:HA3	1.90	1.02
2:D:258:ASP:HB2	2:D:260:GLN:HG2	1.37	1.01
1:A:891:GLY:HA3	1:A:892:GLU:HB2	1.02	1.01
2:B:130:THR:CG2	2:B:210:ALA:HB2	1.91	1.00
2:D:132:ALA:HB1	2:D:186:ALA:HB2	1.47	0.97
2:D:234:ASP:O	2:D:253:LEU:CD1	2.11	0.96
2:B:235:VAL:HG22	2:B:253:LEU:CD1	1.97	0.95
1:A:890:ALA:HB3	1:A:891:GLY:HA2	1.47	0.94
1:C:939:GLY:HA2	1:C:1006:LEU:HD22	1.50	0.92
1:A:1062:THR:HB	1:A:1063:PRO:HD3	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:GLN:C	1:A:889:LYS:CG	2.34	0.91
1:A:891:GLY:N	1:A:892:GLU:HB3	1.85	0.90
2:D:213:LEU:HD12	2:D:218:LEU:CD2	2.02	0.90
2:D:209:ASP:HB2	2:D:211:GLY:CA	2.02	0.89
1:A:889:LYS:NZ	1:A:889:LYS:HB2	1.87	0.88
2:D:54:GLN:HE21	2:D:161:CYS:H	1.20	0.88
2:B:54:GLN:HE21	2:B:161:CYS:H	1.23	0.87
2:D:209:ASP:CB	2:D:211:GLY:N	2.38	0.87
1:A:1000:THR:O	1:A:1004:THR:HG23	1.75	0.86
2:B:130:THR:CG2	2:B:210:ALA:CB	2.53	0.86
2:B:227:ARG:HH11	2:B:227:ARG:HG3	1.39	0.85
2:D:213:LEU:N	2:D:213:LEU:HD23	1.91	0.85
2:B:238:LEU:HD23	2:B:242:LEU:HD12	1.59	0.85
2:B:130:THR:HG21	2:B:210:ALA:HB2	1.56	0.85
1:A:889:LYS:CB	1:A:889:LYS:NZ	2.29	0.85
2:B:234:ASP:O	2:B:238:LEU:HB2	1.75	0.84
1:C:971:GLN:O	1:C:1048:ILE:HG23	1.76	0.84
2:D:234:ASP:CG	2:D:237:ALA:H	1.80	0.84
2:D:232:PHE:HE1	2:D:287:LEU:HD21	1.42	0.84
1:A:889:LYS:HZ3	1:A:889:LYS:HB3	1.42	0.83
2:B:209:ASP:N	2:B:210:ALA:CA	2.38	0.83
2:B:132:ALA:HB1	2:B:186:ALA:HB2	1.59	0.82
2:B:208:THR:C	2:B:210:ALA:HA	1.98	0.82
2:D:209:ASP:CB	2:D:211:GLY:CA	2.57	0.81
2:D:210:ALA:N	2:D:211:GLY:HA3	1.94	0.81
2:B:307:LEU:HD22	2:B:311:ILE:CD1	2.11	0.81
2:B:130:THR:HG22	2:B:210:ALA:HB2	1.60	0.80
2:B:306:MET:HE3	2:B:310:LEU:HG	1.63	0.80
1:C:1060:ARG:HG3	1:C:1060:ARG:NH1	1.93	0.80
1:A:891:GLY:N	1:A:892:GLU:CB	2.43	0.80
2:B:307:LEU:HD22	2:B:311:ILE:HD12	1.64	0.79
2:D:307:LEU:HD22	2:D:311:ILE:CD1	2.12	0.79
2:B:234:ASP:OD1	2:B:237:ALA:HB2	1.82	0.79
1:A:945:ARG:HD2	2:B:120:GLU:OE1	1.83	0.79
2:B:258:ASP:H	2:B:259:GLY:HA2	1.47	0.79
2:D:209:ASP:N	2:D:211:GLY:CA	2.45	0.78
1:A:889:LYS:HB2	1:A:889:LYS:HZ2	1.44	0.78
1:A:888:GLN:C	1:A:889:LYS:HG2	1.94	0.78
2:D:145:GLN:HA	2:D:163:LEU:HD22	1.65	0.78
2:D:128:GLN:HG2	2:D:129:PRO:HD2	1.64	0.78
1:A:997:ILE:HD13	1:C:1022:MET:CE	2.14	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:920:ILE:HG23	1:C:924:LYS:HE3	1.65	0.77
1:A:1062:THR:CB	1:A:1063:PRO:CD	2.45	0.77
1:C:984:VAL:HA	1:C:987:ARG:NH2	2.00	0.77
2:D:209:ASP:HB3	2:D:211:GLY:N	1.98	0.77
2:B:234:ASP:HB3	2:B:237:ALA:HB3	1.66	0.77
2:D:130:THR:HB	2:D:210:ALA:CB	2.14	0.77
2:B:130:THR:HG21	2:B:210:ALA:CB	2.14	0.76
2:B:258:ASP:N	2:B:259:GLY:HA2	1.99	0.76
2:B:234:ASP:O	2:B:238:LEU:CB	2.33	0.76
2:D:55:PHE:HZ	2:D:213:LEU:O	1.67	0.76
2:B:235:VAL:CG2	2:B:253:LEU:HD13	2.12	0.76
1:C:911:LYS:O	1:C:1060:ARG:HD3	1.85	0.75
2:D:209:ASP:H	2:D:211:GLY:HA3	1.49	0.75
2:B:39:LEU:HD12	2:B:169:THR:O	1.86	0.75
1:A:975:LYS:HG2	1:A:978:ARG:NH2	2.01	0.75
2:D:149:GLU:O	2:D:153:ARG:HB3	1.86	0.74
2:B:145:GLN:HA	2:B:163:LEU:HD22	1.69	0.74
1:A:1018:GLN:O	1:A:1022:MET:HG3	1.87	0.74
2:B:227:ARG:NH1	2:B:227:ARG:HG3	2.00	0.74
2:D:145:GLN:HA	2:D:163:LEU:CD2	2.17	0.74
1:A:888:GLN:C	1:A:889:LYS:HG3	2.08	0.73
2:B:235:VAL:HG13	2:B:253:LEU:CD1	2.15	0.73
1:C:900:MET:CE	1:C:904:GLN:HE22	2.01	0.73
2:D:210:ALA:N	2:D:211:GLY:CA	2.50	0.73
2:D:55:PHE:CZ	2:D:213:LEU:O	2.41	0.73
1:A:891:GLY:H	1:A:892:GLU:C	1.92	0.73
2:B:214:THR:OG1	2:B:217:LEU:HD22	1.89	0.73
2:D:54:GLN:NE2	2:D:161:CYS:H	1.86	0.73
2:D:232:PHE:CE1	2:D:287:LEU:CD2	2.70	0.72
1:C:974:ASP:HB2	1:C:1047:LYS:HD3	1.71	0.72
1:C:984:VAL:HA	1:C:987:ARG:CZ	2.19	0.72
2:D:238:LEU:HD23	2:D:242:LEU:HD12	1.71	0.72
1:C:918:ASP:HB3	1:C:964:LEU:HD11	1.71	0.72
1:C:895:ASN:HD22	1:C:898:MET:HB2	1.54	0.72
2:D:64:ARG:HB3	2:D:95:THR:HG22	1.70	0.72
1:C:949:GLN:HG2	2:D:120:GLU:HB2	1.72	0.72
2:D:260:GLN:N	2:D:260:GLN:HE21	1.87	0.71
2:B:225:VAL:HG12	2:B:228:LEU:HD21	1.72	0.71
1:C:913:SER:HB3	1:C:1057:ARG:HH12	1.55	0.71
2:D:209:ASP:H	2:D:211:GLY:CA	2.03	0.71
1:A:935:ARG:NH2	2:B:92:TYR:O	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:SER:HB3	2:B:181:MET:CE	2.20	0.71
2:B:234:ASP:OD1	2:B:237:ALA:CB	2.37	0.71
2:D:209:ASP:HB2	2:D:211:GLY:N	2.04	0.71
1:A:908:GLU:O	1:A:911:LYS:HG3	1.90	0.71
2:D:145:GLN:HE22	2:D:162:PHE:HA	1.55	0.70
2:B:39:LEU:CD1	2:B:44:ILE:HG12	2.21	0.70
1:A:888:GLN:O	1:A:889:LYS:CG	2.29	0.70
2:B:53:ARG:HH11	2:B:53:ARG:HG3	1.57	0.69
2:B:130:THR:HB	2:B:210:ALA:HB3	1.74	0.69
2:B:217:LEU:HD13	2:B:217:LEU:N	2.07	0.69
2:B:40:ASP:O	2:B:44:ILE:HG13	1.93	0.69
2:B:312:ALA:O	2:B:315:ALA:HB3	1.93	0.69
2:D:209:ASP:CB	2:D:211:GLY:HA3	2.22	0.68
2:D:39:LEU:HD12	2:D:169:THR:O	1.93	0.68
2:D:234:ASP:CG	2:D:237:ALA:HB3	2.13	0.68
2:B:234:ASP:CG	2:B:237:ALA:HB3	2.14	0.68
2:D:227:ARG:HG3	2:D:227:ARG:HH11	1.59	0.68
2:B:258:ASP:CB	2:B:260:GLN:HG2	2.16	0.67
2:B:234:ASP:CB	2:B:237:ALA:HB3	2.24	0.67
2:D:312:ALA:O	2:D:315:ALA:HB3	1.93	0.67
2:D:45:ARG:O	2:D:49:GLU:HB2	1.94	0.67
1:C:935:ARG:NH2	2:D:92:TYR:O	2.27	0.67
2:D:307:LEU:HD22	2:D:311:ILE:HD11	1.76	0.67
2:D:39:LEU:CD1	2:D:44:ILE:HG12	2.25	0.67
2:D:245:VAL:HG12	2:D:246:HIS:CE1	2.30	0.67
2:B:125:VAL:O	2:B:126:GLN:HG3	1.95	0.67
1:A:889:LYS:HZ3	1:A:889:LYS:CB	1.99	0.67
2:B:234:ASP:CG	2:B:237:ALA:CB	2.63	0.67
2:B:279:GLN:HG2	2:B:294:VAL:HG12	1.77	0.67
2:D:258:ASP:CB	2:D:260:GLN:HG2	2.20	0.67
2:D:235:VAL:O	2:D:239:CYS:SG	2.53	0.67
2:D:307:LEU:O	2:D:311:ILE:HD12	1.95	0.67
2:D:40:ASP:O	2:D:44:ILE:HG13	1.94	0.67
2:D:227:ARG:HG3	2:D:227:ARG:NH1	2.09	0.66
1:A:895:ASN:HD22	1:A:898:MET:H	1.43	0.66
2:D:132:ALA:HB2	2:D:183:LYS:HA	1.77	0.66
1:C:884:GLU:OE1	1:C:885:PHE:N	2.27	0.66
1:C:906:HIS:O	1:C:910:ARG:HB3	1.95	0.66
1:C:920:ILE:CG2	1:C:924:LYS:HE3	2.25	0.66
1:C:1049:ARG:O	1:C:1049:ARG:HG3	1.95	0.66
2:B:262:LYS:O	2:B:264:PHE:N	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:ALA:O	2:D:317:ALA:N	2.26	0.66
1:C:885:PHE:HD1	1:C:906:HIS:ND1	1.94	0.66
2:B:90:ASP:OD1	2:B:93:LYS:HG3	1.96	0.66
1:A:980:ASN:O	1:A:984:VAL:HG13	1.96	0.66
1:A:886:PRO:HG2	2:B:92:TYR:CE2	2.31	0.66
2:B:114:HIS:CD2	2:B:115:GLN:HG3	2.31	0.65
2:B:213:LEU:N	2:B:213:LEU:HD23	2.11	0.65
2:B:232:PHE:CE1	2:B:234:ASP:HB2	2.31	0.65
1:A:900:MET:HE2	1:A:904:GLN:HE22	1.62	0.65
2:D:234:ASP:OD2	2:D:237:ALA:CB	2.44	0.65
2:D:69:ASP:OD1	2:D:119:ARG:NH2	2.24	0.65
2:D:212:GLN:C	2:D:213:LEU:HD23	2.15	0.65
2:D:234:ASP:OD2	2:D:237:ALA:HB3	1.95	0.65
2:D:257:GLN:OE1	2:D:257:GLN:HA	1.95	0.65
2:D:234:ASP:CG	2:D:237:ALA:CB	2.65	0.65
2:D:153:ARG:HG2	2:D:154:PRO:HD3	1.78	0.65
1:A:900:MET:CE	1:A:904:GLN:HE22	2.10	0.65
2:D:130:THR:HG23	2:D:133:LEU:HB2	1.79	0.64
2:B:245:VAL:HG12	2:B:246:HIS:CE1	2.33	0.64
2:B:54:GLN:NE2	2:B:161:CYS:H	1.95	0.64
1:A:895:ASN:ND2	1:A:898:MET:H	1.95	0.64
2:D:232:PHE:CE2	2:D:238:LEU:HD12	2.33	0.64
1:C:1000:THR:O	1:C:1004:THR:HG23	1.97	0.64
2:D:307:LEU:HD22	2:D:311:ILE:HD12	1.78	0.63
2:B:209:ASP:H	2:B:210:ALA:HA	1.58	0.63
1:C:939:GLY:CA	1:C:1006:LEU:HD22	2.26	0.63
1:A:890:ALA:CB	1:A:891:GLY:HA2	2.19	0.63
1:A:975:LYS:HG2	1:A:978:ARG:HH22	1.64	0.63
2:B:271:THR:HG23	2:B:274:MET:SD	2.39	0.63
2:D:229:PRO:HD2	2:D:232:PHE:CG	2.34	0.62
1:C:900:MET:HE3	1:C:904:GLN:HE22	1.65	0.62
2:B:117:ARG:HA	2:B:121:ARG:O	1.99	0.62
2:B:173:LYS:NZ	2:B:219:HIS:ND1	2.45	0.62
1:A:1044:ALA:O	1:A:1048:ILE:HG12	2.00	0.61
2:D:133:LEU:HD23	2:D:179:GLU:HB2	1.83	0.61
2:D:258:ASP:N	2:D:258:ASP:OD2	2.33	0.61
1:C:911:LYS:HB3	1:C:1060:ARG:HE	1.65	0.61
1:A:1062:THR:O	1:A:1063:PRO:C	2.39	0.60
2:B:53:ARG:NH1	2:B:53:ARG:HG3	2.16	0.60
2:B:52:GLU:O	2:B:56:ARG:HG3	2.01	0.60
2:B:69:ASP:OD1	2:B:119:ARG:NH2	2.21	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:GLU:O	2:B:153:ARG:HB3	2.01	0.60
1:A:911:LYS:O	1:A:1060:ARG:HD3	2.03	0.59
1:C:900:MET:HE2	1:C:904:GLN:HE22	1.66	0.59
1:A:907:ASP:OD1	1:A:910:ARG:NH1	2.35	0.59
2:D:63:ILE:O	2:D:95:THR:HA	2.02	0.59
1:C:988:ILE:N	1:C:989:PRO:HD2	2.17	0.59
2:B:132:ALA:HB2	2:B:183:LYS:HA	1.84	0.59
2:B:46:LYS:HG3	2:B:47:ARG:N	2.18	0.59
2:D:195:GLY:O	2:D:202:THR:HG23	2.02	0.58
2:D:40:ASP:OD1	2:D:41:PRO:HD2	2.03	0.58
2:B:145:GLN:NE2	2:B:163:LEU:H	2.01	0.58
2:B:315:ALA:O	2:B:317:ALA:N	2.33	0.58
1:C:1018:GLN:O	1:C:1022:MET:HG3	2.03	0.58
2:B:208:THR:HG21	2:B:213:LEU:HD21	1.85	0.58
2:B:221:ARG:NH2	2:B:300:GLY:H	2.01	0.58
2:D:209:ASP:C	2:D:211:GLY:HA3	2.24	0.58
2:D:243:SER:OG	2:D:248:PRO:HD2	2.03	0.58
2:D:238:LEU:HD23	2:D:242:LEU:CD1	2.34	0.57
2:B:130:THR:HG23	2:B:133:LEU:HB2	1.86	0.57
2:D:97:PHE:HD2	2:D:128:GLN:NE2	2.01	0.57
1:C:894:ILE:O	1:C:938:ARG:NH1	2.37	0.57
2:B:257:GLN:OE1	2:B:257:GLN:HA	2.04	0.57
2:B:307:LEU:O	2:B:311:ILE:HD12	2.05	0.57
2:D:246:HIS:HB3	2:D:274:MET:HE3	1.86	0.57
2:B:132:ALA:O	2:B:179:GLU:HA	2.04	0.57
2:D:245:VAL:HG12	2:D:246:HIS:ND1	2.20	0.57
2:B:225:VAL:HG22	2:B:294:VAL:HG22	1.86	0.57
2:B:119:ARG:O	2:B:120:GLU:HB2	2.04	0.57
1:C:915:LYS:HB3	1:C:1057:ARG:NH1	2.20	0.56
1:A:942:GLY:HA2	2:B:117:ARG:HH22	1.69	0.56
2:B:250:PHE:HB3	2:B:268:GLU:HB3	1.85	0.56
2:D:134:LEU:HD11	2:D:186:ALA:O	2.04	0.56
2:D:113:PHE:O	2:D:116:SER:HB3	2.04	0.56
2:D:125:VAL:O	2:D:126:GLN:HG3	2.05	0.56
2:B:227:ARG:HH11	2:B:227:ARG:CG	2.15	0.56
2:B:238:LEU:HD23	2:B:242:LEU:CD1	2.33	0.56
2:B:232:PHE:CE2	2:B:238:LEU:HD12	2.40	0.56
2:D:235:VAL:HB	2:D:236:ASP:OD2	2.05	0.56
2:B:153:ARG:N	2:B:154:PRO:HD2	2.21	0.56
2:D:214:THR:OG1	2:D:217:LEU:HD22	2.05	0.56
1:C:967:GLU:OE1	1:C:967:GLU:HA	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:O	2:B:95:THR:HA	2.07	0.55
1:C:895:ASN:HD22	1:C:898:MET:H	1.54	0.55
2:B:315:ALA:C	2:B:317:ALA:H	2.09	0.55
2:D:229:PRO:O	2:D:232:PHE:HB3	2.07	0.55
2:B:302:PRO:HD2	2:B:305:SER:OG	2.07	0.55
1:A:984:VAL:HA	1:A:987:ARG:CZ	2.37	0.55
2:D:209:ASP:HB2	2:D:211:GLY:HA2	1.87	0.55
2:B:42:GLU:HA	2:B:42:GLU:OE2	2.06	0.55
2:D:157:SER:HB3	2:D:181:MET:CE	2.36	0.55
2:D:67:PRO:HB3	2:D:119:ARG:NH2	2.22	0.55
1:C:919:ILE:HG13	1:C:964:LEU:CD1	2.37	0.54
1:C:885:PHE:HD1	1:C:906:HIS:CG	2.25	0.54
2:D:130:THR:CB	2:D:210:ALA:HB2	2.23	0.54
2:B:226:ASP:O	2:B:227:ARG:HB2	2.06	0.54
2:D:246:HIS:CD2	2:D:274:MET:HG2	2.42	0.54
2:D:228:LEU:HD23	2:D:292:LEU:HD22	1.87	0.54
1:C:981:LEU:HD12	1:C:1040:GLU:HB2	1.88	0.54
2:B:157:SER:HB3	2:B:181:MET:HE2	1.89	0.54
1:A:893:VAL:C	1:A:894:ILE:CG2	2.70	0.54
2:B:145:GLN:HE22	2:B:162:PHE:HA	1.72	0.54
1:A:891:GLY:H	1:A:892:GLU:CA	2.21	0.54
2:B:145:GLN:HE22	2:B:163:LEU:H	1.55	0.54
2:D:213:LEU:HB2	2:D:218:LEU:HD23	1.90	0.54
2:B:307:LEU:HD22	2:B:311:ILE:HD11	1.86	0.54
2:D:128:GLN:CG	2:D:129:PRO:HD2	2.37	0.53
2:B:45:ARG:CG	2:B:45:ARG:HH21	2.22	0.53
2:D:157:SER:HB2	2:D:181:MET:HG3	1.90	0.53
1:A:1035:LYS:HE3	1:A:1039:ARG:HH12	1.73	0.53
1:C:1042:GLU:HB2	1:C:1058:TRP:CZ3	2.44	0.53
2:D:86:TYR:HB3	2:D:99:THR:CB	2.39	0.53
2:B:232:PHE:CE1	2:B:287:LEU:HD21	2.44	0.53
1:A:920:ILE:O	1:A:924:LYS:HG3	2.09	0.53
1:C:887:GLU:HA	1:C:903:ARG:HH12	1.73	0.53
2:B:258:ASP:N	2:B:258:ASP:OD2	2.41	0.52
2:D:317:ALA:O	2:D:318:LEU:O	2.27	0.52
2:B:39:LEU:HD12	2:B:44:ILE:HG12	1.89	0.52
2:D:132:ALA:HB1	2:D:186:ALA:CB	2.32	0.52
2:B:133:LEU:HD23	2:B:179:GLU:HB2	1.91	0.52
2:B:213:LEU:HD12	2:B:218:LEU:CD2	2.40	0.52
2:D:225:VAL:HG22	2:D:294:VAL:HG22	1.91	0.52
2:B:235:VAL:CG2	2:B:253:LEU:CD1	2.80	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:LEU:HD23	2:D:267:LEU:N	2.25	0.52
2:D:213:LEU:HD12	2:D:218:LEU:HD21	1.87	0.52
1:C:911:LYS:HB3	1:C:1060:ARG:NE	2.25	0.52
2:D:86:TYR:HB3	2:D:99:THR:HB	1.92	0.52
1:A:984:VAL:HA	1:A:987:ARG:NH2	2.24	0.52
1:A:891:GLY:H	1:A:892:GLU:HB3	1.70	0.52
1:A:1060:ARG:HD2	1:A:1062:THR:HG23	1.92	0.52
1:C:913:SER:HB3	1:C:1057:ARG:NH1	2.24	0.52
1:A:891:GLY:N	1:A:892:GLU:CA	2.73	0.52
1:C:1011:ILE:HD11	1:C:1015:GLU:HB3	1.91	0.52
1:C:905:LEU:HD21	1:C:1034:VAL:HG11	1.92	0.51
1:C:980:ASN:O	1:C:984:VAL:HG13	2.10	0.51
2:D:153:ARG:HG2	2:D:154:PRO:CD	2.41	0.51
2:B:225:VAL:CG1	2:B:228:LEU:HD21	2.39	0.51
2:B:243:SER:O	2:B:245:VAL:N	2.43	0.51
2:B:246:HIS:HB3	2:B:274:MET:HE3	1.92	0.51
1:A:997:ILE:HD13	1:C:1022:MET:HE1	1.93	0.51
1:A:886:PRO:O	1:A:903:ARG:NH1	2.43	0.51
2:B:236:ASP:O	2:B:240:ARG:HB2	2.10	0.51
2:D:232:PHE:HE2	2:D:238:LEU:HD12	1.76	0.51
1:C:1042:GLU:HB2	1:C:1058:TRP:CH2	2.45	0.51
2:B:210:ALA:O	2:B:212:GLN:NE2	2.44	0.51
2:D:39:LEU:HD13	2:D:44:ILE:HG12	1.91	0.51
1:C:906:HIS:CE1	1:C:910:ARG:HD3	2.46	0.51
2:B:130:THR:CG2	2:B:210:ALA:HB3	2.41	0.51
2:D:102:ASN:OD1	2:D:104:GLU:HB2	2.11	0.51
1:C:949:GLN:HE21	2:D:120:GLU:HG3	1.77	0.50
1:C:914:SER:HB3	1:C:921:ALA:HB2	1.93	0.50
1:C:972:CYS:O	1:C:978:ARG:NH2	2.44	0.50
2:D:227:ARG:CG	2:D:227:ARG:HH11	2.21	0.50
2:B:232:PHE:CZ	2:B:234:ASP:CB	2.95	0.50
1:A:1008:ARG:O	1:A:1011:ILE:HG22	2.11	0.50
2:B:39:LEU:HD13	2:B:44:ILE:HG12	1.91	0.50
2:B:266:VAL:C	2:B:267:LEU:HD23	2.31	0.50
2:B:235:VAL:CG1	2:B:253:LEU:HD12	2.25	0.50
2:D:42:GLU:OE2	2:D:42:GLU:HA	2.10	0.50
1:C:1044:ALA:O	1:C:1048:ILE:HG12	2.12	0.49
1:A:893:VAL:HG12	1:A:938:ARG:CZ	2.42	0.49
1:A:1035:LYS:HE3	1:A:1039:ARG:NH1	2.26	0.49
2:B:84:LEU:HD22	2:B:100:LEU:CD2	2.42	0.49
2:D:204:TYR:CE2	2:D:206:HIS:HB3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:895:ASN:HD22	1:C:898:MET:CB	2.23	0.49
2:D:266:VAL:C	2:D:267:LEU:HD23	2.33	0.49
1:C:981:LEU:HD13	1:C:1041:ALA:N	2.28	0.49
2:D:209:ASP:HB3	2:D:210:ALA:C	2.32	0.49
2:D:67:PRO:CB	2:D:119:ARG:NH2	2.76	0.49
1:C:913:SER:CB	1:C:1057:ARG:HH12	2.22	0.49
2:D:242:LEU:HD13	2:D:267:LEU:HD11	1.94	0.49
2:D:86:TYR:HB3	2:D:99:THR:OG1	2.12	0.49
2:D:234:ASP:CG	2:D:237:ALA:N	2.56	0.48
1:C:915:LYS:O	1:C:1057:ARG:HB3	2.13	0.48
2:B:110:ILE:HD13	2:B:126:GLN:HA	1.94	0.48
2:B:256:GLY:HA3	2:B:262:LYS:HE2	1.95	0.48
2:D:153:ARG:N	2:D:154:PRO:HD2	2.28	0.48
2:B:153:ARG:HG2	2:B:154:PRO:HD3	1.94	0.48
2:D:232:PHE:CD2	2:D:232:PHE:C	2.87	0.48
1:C:885:PHE:CE2	2:D:92:TYR:CD1	3.00	0.48
2:D:217:LEU:N	2:D:217:LEU:HD13	2.28	0.48
1:A:1011:ILE:HD11	1:A:1015:GLU:HB3	1.96	0.48
2:D:234:ASP:OD2	2:D:237:ALA:HB2	2.12	0.48
1:A:1062:THR:OG1	1:A:1063:PRO:HD2	2.13	0.48
2:B:213:LEU:HD12	2:B:218:LEU:HD21	1.95	0.48
2:D:318:LEU:C	2:D:318:LEU:HD22	2.34	0.48
1:A:945:ARG:NH1	2:B:120:GLU:OE2	2.47	0.48
1:C:908:GLU:O	1:C:911:LYS:HG3	2.14	0.48
2:B:234:ASP:CG	2:B:237:ALA:HB2	2.30	0.48
1:C:887:GLU:O	1:C:888:GLN:HB3	2.14	0.48
2:B:130:THR:HG22	2:B:210:ALA:CB	2.30	0.48
2:B:130:THR:CB	2:B:210:ALA:HB3	2.42	0.48
1:C:908:GLU:OE2	1:C:1039:ARG:HG2	2.14	0.48
2:D:271:THR:HG23	2:D:274:MET:SD	2.54	0.47
2:B:314:GLN:O	2:B:314:GLN:HG2	2.14	0.47
2:B:93:LYS:HB3	2:B:93:LYS:HE2	1.62	0.47
2:D:132:ALA:HA	2:D:207:TRP:HZ3	1.79	0.47
1:C:918:ASP:CB	1:C:964:LEU:HD11	2.44	0.47
2:B:250:PHE:CD1	2:B:251:CYS:N	2.82	0.47
2:B:45:ARG:HG3	2:B:45:ARG:NH2	2.29	0.47
2:D:44:ILE:HD13	2:D:168:ARG:O	2.14	0.47
1:A:983:GLN:O	1:A:985:CYS:N	2.47	0.47
1:A:983:GLN:C	1:A:985:CYS:H	2.18	0.47
2:D:70:VAL:HA	2:D:74:GLU:OE2	2.15	0.47
2:D:39:LEU:HD13	2:D:44:ILE:CG1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:SER:HA	2:B:246:HIS:O	2.14	0.47
2:B:135:CYS:SG	2:B:298:ALA:HB1	2.54	0.47
1:C:915:LYS:CB	1:C:1057:ARG:NH1	2.78	0.47
2:B:282:ALA:O	2:B:285:LEU:HB2	2.15	0.47
1:A:1014:GLU:HG3	1:A:1014:GLU:H	1.56	0.47
1:C:1060:ARG:CG	1:C:1060:ARG:HH11	2.05	0.46
2:D:212:GLN:CA	2:D:213:LEU:HD23	2.45	0.46
2:B:157:SER:HB3	2:B:181:MET:HE3	1.96	0.46
2:D:39:LEU:HD12	2:D:44:ILE:HG12	1.95	0.46
1:A:894:ILE:O	1:A:938:ARG:NH1	2.48	0.46
1:C:905:LEU:HD21	1:C:1034:VAL:CG1	2.45	0.46
1:C:885:PHE:CE2	2:D:92:TYR:HD1	2.33	0.46
1:A:894:ILE:HG21	1:A:894:ILE:HD13	1.35	0.46
2:B:258:ASP:N	2:B:259:GLY:CA	2.75	0.46
1:C:1020:THR:O	1:C:1024:VAL:HG23	2.15	0.46
1:C:981:LEU:CD1	1:C:1040:GLU:HB2	2.46	0.46
1:A:900:MET:CE	1:A:904:GLN:NE2	2.78	0.46
2:D:221:ARG:HB2	2:D:221:ARG:HE	1.55	0.46
2:B:131:ASP:HB3	2:B:132:ALA:H	1.56	0.46
1:C:1044:ALA:O	1:C:1048:ILE:HD11	2.15	0.46
2:B:39:LEU:HD13	2:B:44:ILE:CG1	2.46	0.46
2:B:128:GLN:CG	2:B:129:PRO:HD2	2.45	0.46
2:D:213:LEU:HD12	2:D:218:LEU:HD22	1.93	0.46
2:D:85:LYS:N	2:D:99:THR:O	2.46	0.46
1:C:983:GLN:C	1:C:985:CYS:H	2.19	0.46
1:C:972:CYS:HA	1:C:1048:ILE:HD13	1.98	0.45
2:B:42:GLU:OE1	2:B:45:ARG:NH2	2.50	0.45
1:A:893:VAL:HG23	1:A:893:VAL:H	1.48	0.45
2:D:93:LYS:HB3	2:D:93:LYS:HE2	1.55	0.45
2:B:212:GLN:H	2:B:212:GLN:CD	2.20	0.45
1:A:920:ILE:CG2	1:A:924:LYS:HE3	2.46	0.45
1:A:997:ILE:HD13	1:C:1022:MET:HE2	1.98	0.45
2:B:40:ASP:OD1	2:B:41:PRO:HD2	2.16	0.45
2:D:130:THR:HB	2:D:210:ALA:CA	2.45	0.45
1:A:884:GLU:HG2	1:A:910:ARG:CZ	2.47	0.45
1:C:885:PHE:CD1	1:C:906:HIS:CG	3.04	0.45
1:C:949:GLN:CG	2:D:120:GLU:HB2	2.45	0.45
2:D:243:SER:HA	2:D:246:HIS:O	2.16	0.45
2:B:45:ARG:CG	2:B:45:ARG:NH2	2.79	0.45
2:B:222:CYS:HA	2:B:267:LEU:O	2.17	0.45
1:C:1035:LYS:HE3	1:C:1039:ARG:NH1	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:LEU:HD23	2:B:267:LEU:N	2.31	0.44
2:B:85:LYS:HD3	2:B:85:LYS:HA	1.88	0.44
1:C:1031:MET:CE	1:C:1031:MET:HA	2.48	0.44
2:D:260:GLN:N	2:D:260:GLN:NE2	2.63	0.44
2:D:157:SER:HB3	2:D:181:MET:HE2	1.99	0.44
2:D:157:SER:HB3	2:D:181:MET:HE3	2.00	0.44
1:A:1022:MET:CE	1:C:997:ILE:HD13	2.48	0.44
2:D:260:GLN:CA	2:D:260:GLN:NE2	2.79	0.44
2:B:145:GLN:HA	2:B:163:LEU:CD2	2.43	0.44
2:D:250:PHE:HB3	2:D:268:GLU:HB3	1.99	0.44
2:B:235:VAL:CG1	2:B:253:LEU:CD1	2.93	0.44
2:B:228:LEU:HD23	2:B:292:LEU:HD22	1.99	0.44
2:B:114:HIS:O	2:B:115:GLN:HB2	2.16	0.44
1:C:885:PHE:CD1	1:C:906:HIS:ND1	2.82	0.44
2:D:246:HIS:HB3	2:D:274:MET:CE	2.48	0.44
2:D:182:LYS:HD2	2:D:182:LYS:HA	1.52	0.44
2:B:71:THR:O	2:B:74:GLU:HB2	2.18	0.44
1:A:895:ASN:HD22	1:A:898:MET:HB2	1.83	0.44
2:B:226:ASP:O	2:B:227:ARG:CB	2.65	0.43
1:C:895:ASN:ND2	1:C:898:MET:HB2	2.27	0.43
1:A:990:THR:O	1:A:994:GLN:HG3	2.17	0.43
2:B:106:ALA:O	2:B:110:ILE:HG13	2.18	0.43
2:B:245:VAL:HG12	2:B:246:HIS:ND1	2.33	0.43
2:D:194:LEU:HA	2:D:205:VAL:HG23	2.00	0.43
2:B:182:LYS:HA	2:B:182:LYS:HD2	1.68	0.43
2:B:48:LEU:HD23	2:B:48:LEU:HA	1.64	0.43
2:B:139:LEU:HD23	2:B:203:LEU:HD22	1.99	0.43
1:C:956:LYS:O	1:C:959:ASP:HB2	2.19	0.43
2:D:106:ALA:O	2:D:110:ILE:HG13	2.19	0.43
2:B:212:GLN:N	2:B:212:GLN:CD	2.71	0.43
2:D:40:ASP:CG	2:D:41:PRO:HD2	2.38	0.43
1:A:893:VAL:C	1:A:894:ILE:HG23	2.31	0.43
2:D:279:GLN:HG2	2:D:294:VAL:HG12	2.00	0.43
1:A:918:ASP:CB	1:A:964:LEU:HD11	2.49	0.43
1:C:1014:GLU:HG3	1:C:1014:GLU:H	1.56	0.43
1:C:975:LYS:HA	1:C:975:LYS:HD2	1.28	0.43
2:D:47:ARG:NH2	2:D:170:GLY:O	2.46	0.43
2:D:221:ARG:NH2	2:D:300:GLY:H	2.16	0.43
2:B:235:VAL:O	2:B:239:CYS:SG	2.76	0.43
2:D:315:ALA:C	2:D:317:ALA:H	2.16	0.43
1:A:920:ILE:HA	1:A:920:ILE:HD13	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:ARG:HD3	2:D:160:ARG:CZ	2.49	0.43
2:B:238:LEU:CD2	2:B:242:LEU:CD1	2.97	0.43
1:C:1044:ALA:O	1:C:1048:ILE:CG1	2.67	0.43
1:C:983:GLN:O	1:C:985:CYS:N	2.52	0.42
1:C:912:TRP:CD1	1:C:920:ILE:HD11	2.54	0.42
1:A:1001:VAL:CG2	1:C:1001:VAL:CG2	2.97	0.42
1:A:967:GLU:HA	1:A:967:GLU:OE1	2.19	0.42
2:B:157:SER:O	2:B:181:MET:HG2	2.19	0.42
1:A:938:ARG:HD2	1:A:938:ARG:HA	1.82	0.42
2:D:42:GLU:O	2:D:46:LYS:HB3	2.19	0.42
2:D:311:ILE:HG22	2:D:312:ALA:N	2.33	0.42
2:B:246:HIS:CD2	2:B:274:MET:HG2	2.55	0.42
2:B:238:LEU:CD2	2:B:242:LEU:HD12	2.40	0.42
1:C:925:ARG:HG2	2:D:69:ASP:HB2	2.01	0.42
2:D:250:PHE:O	2:D:251:CYS:HB2	2.18	0.42
1:A:883:GLU:O	1:A:906:HIS:HE1	2.03	0.42
2:D:222:CYS:HA	2:D:267:LEU:O	2.18	0.42
2:D:97:PHE:HD2	2:D:128:GLN:HE21	1.67	0.42
1:C:900:MET:HE3	1:C:904:GLN:NE2	2.30	0.42
2:B:49:GLU:HG2	2:B:53:ARG:HH12	1.83	0.42
1:A:900:MET:HE3	1:A:904:GLN:NE2	2.35	0.42
1:C:1002:LYS:NZ	1:C:1020:THR:OG1	2.37	0.42
2:D:145:GLN:CA	2:D:163:LEU:CD2	2.95	0.42
2:D:190:LYS:HA	2:D:205:VAL:HG11	2.02	0.42
2:D:64:ARG:HG3	2:D:124:SER:HB3	2.02	0.42
1:C:933:MET:O	1:C:937:VAL:HB	2.19	0.42
2:B:238:LEU:HD23	2:B:238:LEU:C	2.40	0.42
1:C:919:ILE:HG13	1:C:964:LEU:HD13	2.01	0.42
1:C:895:ASN:ND2	1:C:897:PRO:HD2	2.34	0.42
2:B:232:PHE:C	2:B:232:PHE:CD2	2.93	0.42
2:D:226:ASP:O	2:D:227:ARG:HB2	2.20	0.42
1:C:953:ASP:O	1:C:956:LYS:N	2.53	0.42
1:A:981:LEU:HD13	1:A:1040:GLU:HB2	2.01	0.42
2:B:44:ILE:HD13	2:B:168:ARG:O	2.20	0.41
2:D:228:LEU:HD23	2:D:292:LEU:CD2	2.49	0.41
1:C:968:VAL:HG21	1:C:1056:LEU:HD12	2.02	0.41
2:B:221:ARG:HH22	2:B:300:GLY:H	1.68	0.41
2:D:210:ALA:CA	2:D:211:GLY:C	2.88	0.41
2:B:84:LEU:CD2	2:B:100:LEU:CD2	2.97	0.41
1:A:968:VAL:HG23	1:A:1054:PHE:HE2	1.86	0.41
1:C:945:ARG:HD2	2:D:120:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:LEU:HA	2:D:198:LEU:HD23	1.84	0.41
2:D:213:LEU:HB2	2:D:218:LEU:CD2	2.50	0.41
2:B:194:LEU:CD1	2:B:205:VAL:H	2.34	0.41
1:A:887:GLU:H	1:A:887:GLU:HG3	1.57	0.41
2:D:132:ALA:O	2:D:179:GLU:HA	2.21	0.41
2:B:253:LEU:HD23	2:B:261:LEU:HD22	2.03	0.41
2:B:45:ARG:O	2:B:49:GLU:HB2	2.21	0.41
2:D:195:GLY:HA2	2:D:202:THR:CG2	2.50	0.41
1:A:1011:ILE:HD13	1:A:1012:SER:O	2.21	0.41
2:D:46:LYS:HG3	2:D:47:ARG:N	2.30	0.41
2:D:146:GLN:O	2:D:146:GLN:HG2	2.21	0.41
2:B:235:VAL:O	2:B:239:CYS:HB2	2.21	0.40
1:C:984:VAL:CA	1:C:987:ARG:NH2	2.79	0.40
2:D:140:PRO:HA	2:D:141:PRO:HD3	1.99	0.40
2:B:208:THR:C	2:B:210:ALA:CA	2.80	0.40
2:B:232:PHE:HE2	2:B:238:LEU:HD12	1.86	0.40
1:A:1011:ILE:HD11	1:A:1015:GLU:CB	2.52	0.40
2:D:157:SER:CB	2:D:181:MET:HE3	2.52	0.40
2:D:52:GLU:O	2:D:56:ARG:HG3	2.22	0.40
1:A:951:ALA:HB2	1:A:999:SER:OG	2.21	0.40
2:B:92:TYR:O	2:B:92:TYR:CG	2.75	0.40
1:A:1008:ARG:H	1:A:1008:ARG:HG2	1.64	0.40
2:D:84:LEU:CD2	2:D:100:LEU:CD2	2.99	0.40
2:B:300:GLY:HA3	2:B:301:PRO:HD3	1.90	0.40
2:D:113:PHE:HA	2:D:116:SER:HB3	2.03	0.40
2:B:84:LEU:HD22	2:B:100:LEU:HD23	2.03	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	180/188 (96%)	167 (93%)	9 (5%)	4 (2%)	8 24
1	C	168/188 (89%)	159 (95%)	8 (5%)	1 (1%)	30 62
2	B	277/283 (98%)	256 (92%)	17 (6%)	4 (1%)	14 38
2	D	278/283 (98%)	258 (93%)	16 (6%)	4 (1%)	14 38
All	All	903/942 (96%)	840 (93%)	50 (6%)	13 (1%)	14 38

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	892	GLU
1	A	984	VAL
2	B	263	GLY
2	B	316	THR
2	D	260	GLN
2	B	244	ALA
1	C	984	VAL
2	D	316	THR
2	D	244	ALA
1	A	889	LYS
1	A	891	GLY
2	D	251	CYS
2	B	260	GLN

5.3.2 Protein sidechains (i)

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	153/159 (96%)	119 (78%)	34 (22%)	1 3
1	C	149/159 (94%)	119 (80%)	30 (20%)	1 4
2	B	230/233 (99%)	185 (80%)	45 (20%)	1 4
2	D	231/233 (99%)	178 (77%)	53 (23%)	1 2
All	All	763/784 (97%)	601 (79%)	162 (21%)	1 3

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	883	GLU
1	A	884	GLU
1	A	885	PHE
1	A	887	GLU
1	A	888	GLN
1	A	892	GLU
1	A	893	VAL
1	A	895	ASN
1	A	898	MET
1	A	904	GLN
1	A	910	ARG
1	A	911	LYS
1	A	915	LYS
1	A	928	LEU
1	A	934	SER
1	A	937	VAL
1	A	944	LYS
1	A	970	LYS
1	A	975	LYS
1	A	985	CYS
1	A	986	GLU
1	A	987	ARG
1	A	1008	ARG
1	A	1009	THR
1	A	1010	ASN
1	A	1011	ILE
1	A	1014	GLU
1	A	1017	GLU
1	A	1046	ILE
1	A	1047	LYS
1	A	1049	ARG
1	A	1050	THR
1	A	1060	ARG
1	A	1061	LYS
2	B	39	LEU
2	B	40	ASP
2	B	45	ARG
2	B	46	LYS
2	B	56	ARG
2	B	64	ARG
2	B	83	GLU
2	B	93	LYS
2	B	107	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	124	SER
2	B	131	ASP
2	B	133	LEU
2	B	149	GLU
2	B	152	VAL
2	B	157	SER
2	B	163	LEU
2	B	166	SER
2	B	168	ARG
2	B	181	MET
2	B	183	LYS
2	B	184	ASP
2	B	198	LEU
2	B	206	HIS
2	B	209	ASP
2	B	213	LEU
2	B	217	LEU
2	B	221	ARG
2	B	227	ARG
2	B	232	PHE
2	B	234	ASP
2	B	235	VAL
2	B	240	ARG
2	B	247	SER
2	B	249	THR
2	B	252	GLN
2	B	257	GLN
2	B	258	ASP
2	B	267	LEU
2	B	271	THR
2	B	285	LEU
2	B	295	SER
2	B	304	ARG
2	B	305	SER
2	B	307	LEU
2	B	314	GLN
1	C	883	GLU
1	C	884	GLU
1	C	885	PHE
1	C	892	GLU
1	C	896	GLN
1	C	904	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	905	LEU
1	C	911	LYS
1	C	915	LYS
1	C	928	LEU
1	C	934	SER
1	C	937	VAL
1	C	963	ARG
1	C	975	LYS
1	C	985	CYS
1	C	986	GLU
1	C	987	ARG
1	C	1008	ARG
1	C	1009	THR
1	C	1010	ASN
1	C	1011	ILE
1	C	1014	GLU
1	C	1017	GLU
1	C	1033	SER
1	C	1046	ILE
1	C	1047	LYS
1	C	1049	ARG
1	C	1060	ARG
1	C	1061	LYS
1	C	1063	PRO
2	D	39	LEU
2	D	45	ARG
2	D	46	LYS
2	D	56	ARG
2	D	64	ARG
2	D	83	GLU
2	D	93	LYS
2	D	104	GLU
2	D	107	GLU
2	D	116	SER
2	D	124	SER
2	D	133	LEU
2	D	149	GLU
2	D	152	VAL
2	D	153	ARG
2	D	163	LEU
2	D	166	SER
2	D	168	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	181	MET
2	D	182	LYS
2	D	183	LYS
2	D	184	ASP
2	D	191	SER
2	D	198	LEU
2	D	206	HIS
2	D	209	ASP
2	D	212	GLN
2	D	213	LEU
2	D	217	LEU
2	D	221	ARG
2	D	227	ARG
2	D	232	PHE
2	D	234	ASP
2	D	247	SER
2	D	249	THR
2	D	252	GLN
2	D	253	LEU
2	D	255	CYS
2	D	257	GLN
2	D	258	ASP
2	D	260	GLN
2	D	267	LEU
2	D	271	THR
2	D	285	LEU
2	D	290	SER
2	D	293	ARG
2	D	295	SER
2	D	304	ARG
2	D	305	SER
2	D	307	LEU
2	D	311	ILE
2	D	314	GLN
2	D	318	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	895	ASN
1	A	904	GLN
1	A	906	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	980	ASN
1	A	983	GLN
1	A	1010	ASN
1	A	1026	ASN
1	A	1029	ASN
2	B	54	GLN
2	B	76	HIS
2	B	145	GLN
2	B	206	HIS
2	B	212	GLN
2	B	246	HIS
2	B	260	GLN
1	C	888	GLN
1	C	895	ASN
1	C	904	GLN
1	C	949	GLN
1	C	980	ASN
1	C	983	GLN
1	C	1026	ASN
1	C	1029	ASN
2	D	54	GLN
2	D	145	GLN
2	D	206	HIS
2	D	212	GLN
2	D	246	HIS
2	D	260	GLN

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

There are no ligands in this entry.

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^{th} 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	182/188 (96%)	0.28	8 (4%) 38 31	23, 43, 91, 111	0
1	C	174/188 (92%)	0.98	23 (13%) 4 3	48, 69, 112, 135	0
2	B	279/283 (98%)	0.29	8 (2%) 55 48	32, 55, 96, 126	0
2	D	280/283 (98%)	0.55	19 (6%) 20 15	44, 69, 108, 137	0
All	All	915/942 (97%)	0.50	58 (6%) 23 17	23, 61, 102, 137	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	213	LEU	7.0
1	C	965	ALA	6.5
1	C	1038	VAL	6.4
2	D	238	LEU	5.9
1	C	961	VAL	5.6
2	D	211	GLY	5.5
2	B	234	ASP	5.5
1	C	971	GLN	5.4
1	A	1063	PRO	5.3
2	D	209	ASP	5.3
1	C	1046	ILE	4.5
1	A	891	GLY	4.3
1	C	968	VAL	4.3
2	D	235	VAL	4.1
2	B	210	ALA	3.9
1	C	1048	ILE	3.7
2	B	209	ASP	3.6
1	A	1009	THR	3.5
2	D	168	ARG	3.4
2	D	221	ARG	3.4
2	D	265	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	973	THR	3.3
2	D	232	PHE	3.1
1	C	1049	ARG	3.1
1	C	966	LYS	3.1
2	B	304	ARG	3.1
2	D	267	LEU	2.8
1	C	985	CYS	2.8
2	B	242	LEU	2.7
1	C	1057	ARG	2.7
2	D	218	LEU	2.7
2	D	266	VAL	2.7
1	C	977	ILE	2.7
2	D	68	GLY	2.7
1	C	884	GLU	2.6
1	C	999	SER	2.6
2	D	210	ALA	2.6
1	C	967	GLU	2.5
2	D	214	THR	2.5
1	C	1041	ALA	2.5
1	C	981	LEU	2.5
2	D	270	GLU	2.5
1	C	1045	SER	2.5
2	B	213	LEU	2.5
1	C	1039	ARG	2.4
1	A	1062	THR	2.4
1	A	1010	ASN	2.3
1	A	1008	ARG	2.3
2	D	242	LEU	2.3
1	C	927	ALA	2.3
2	B	216	ALA	2.3
1	C	1034	VAL	2.3
1	A	936	LEU	2.2
1	A	890	ALA	2.2
2	D	162	PHE	2.2
1	C	1032	GLN	2.1
2	B	238	LEU	2.1
2	D	272	ALA	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.