



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:09 AM GMT

PDB ID : 3HBL
Title : Crystal Structure of S. aureus Pyruvate Carboxylase T908A Mutant
Authors : Tong, L.; Yu, L.P.C.
Deposited on : 2009-05-04
Resolution : 2.71 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

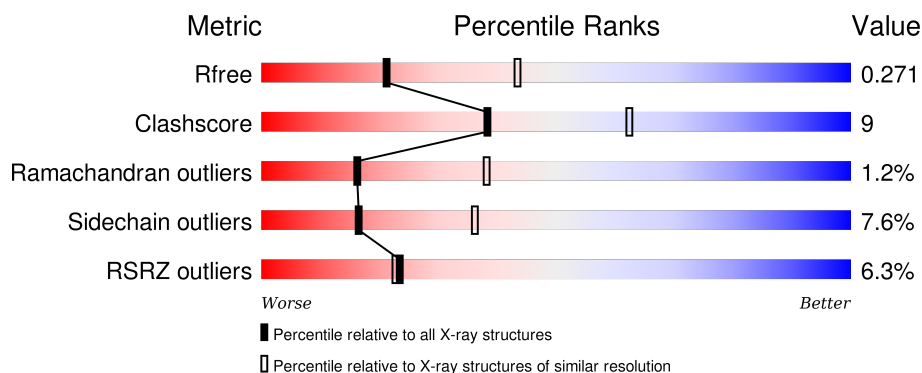
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1150	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	1150	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	C	1150	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 7%</div> </div> </div>
1	D	1150	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>• 7%</div> </div> </div>

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
3	MN	C	2002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34327 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.

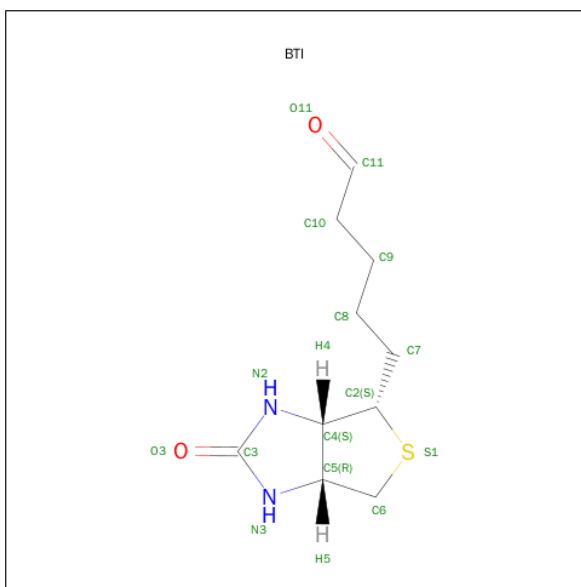
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1131	Total	C	N	O	S	0	0	0
			8923	5654	1502	1737	30			
1	B	1074	Total	C	N	O	S	0	0	0
			8463	5364	1427	1643	29			
1	C	1067	Total	C	N	O	S	0	0	0
			8439	5349	1421	1639	30			
1	D	1067	Total	C	N	O	S	0	0	0
			8411	5333	1416	1633	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	908	ALA	THR	ENGINEERED	UNP Q99UY8
B	908	ALA	THR	ENGINEERED	UNP Q99UY8
C	908	ALA	THR	ENGINEERED	UNP Q99UY8
D	908	ALA	THR	ENGINEERED	UNP Q99UY8

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

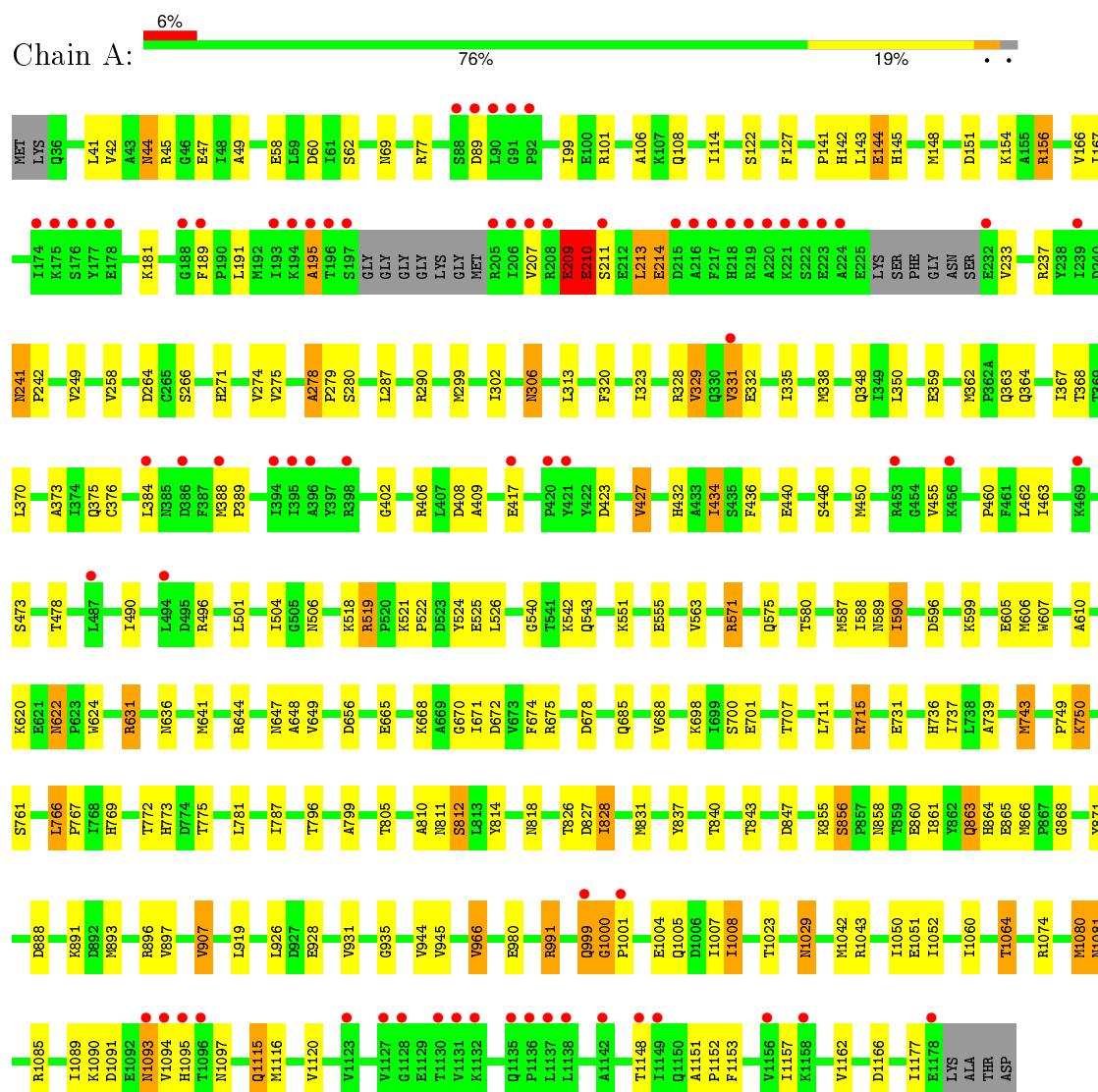


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

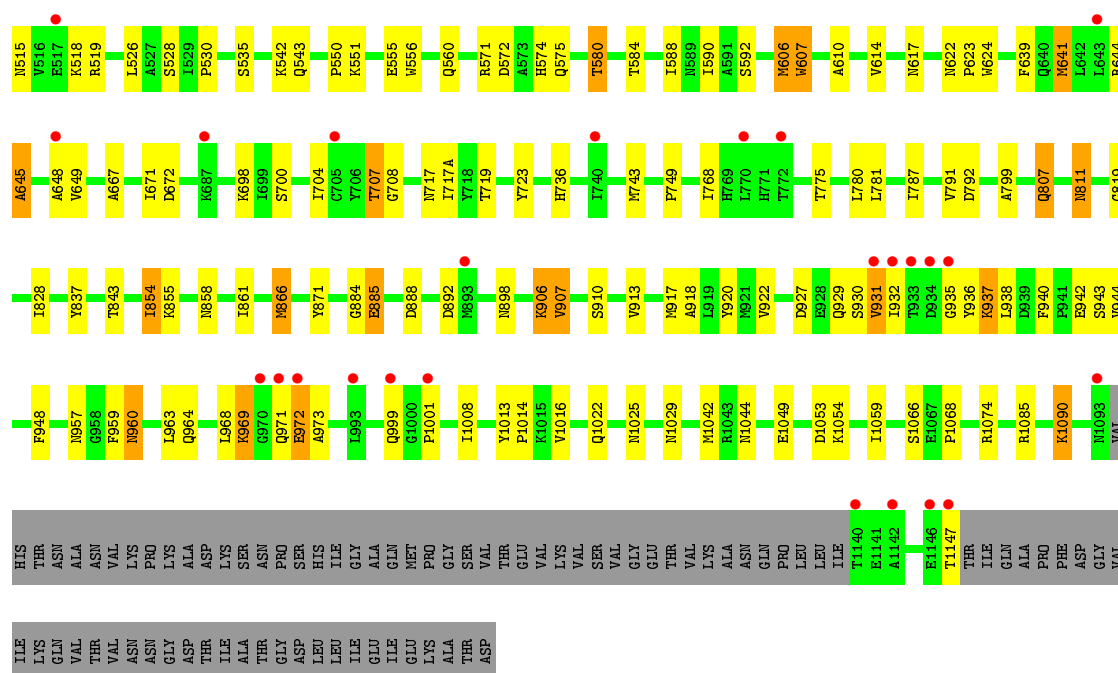
• Molecule 1: Pyruvate carboxylase



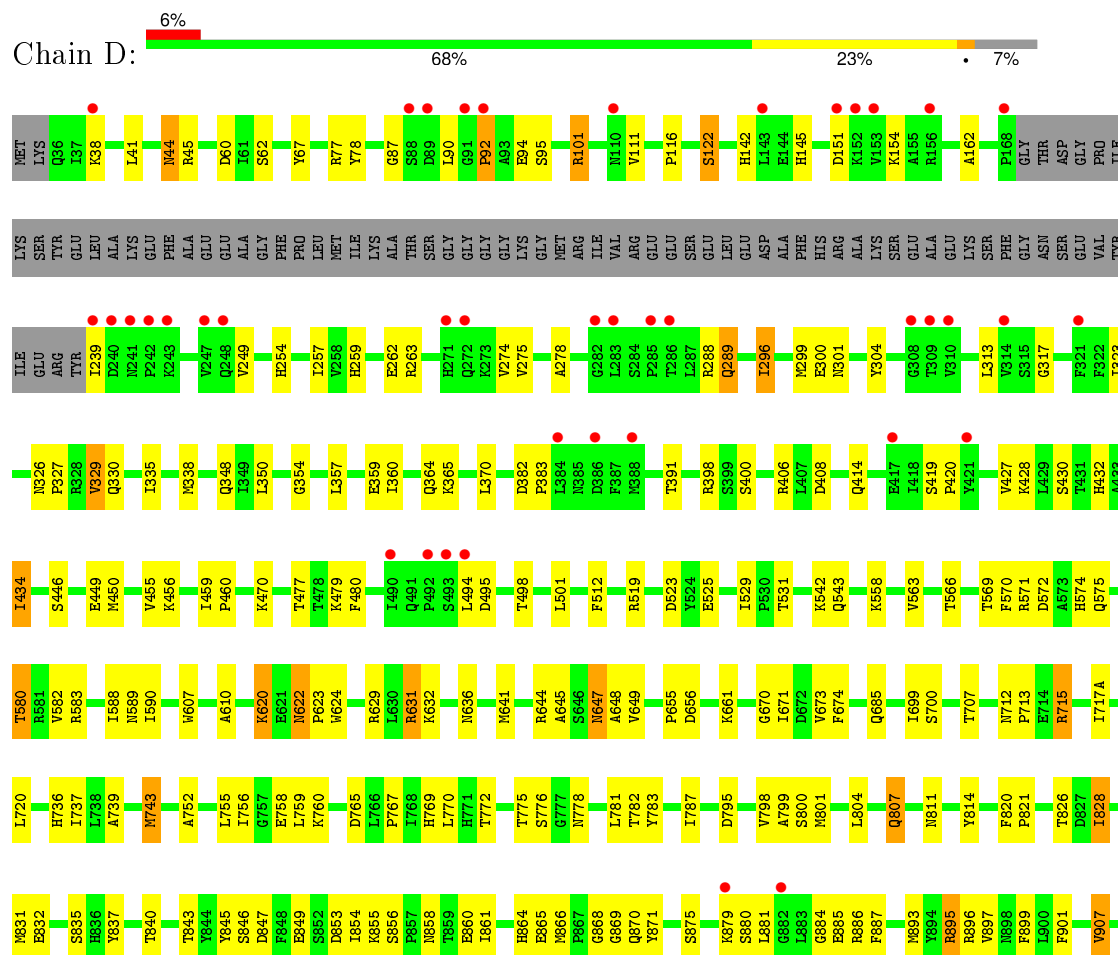
• Molecule 1: Pyruvate carboxylase

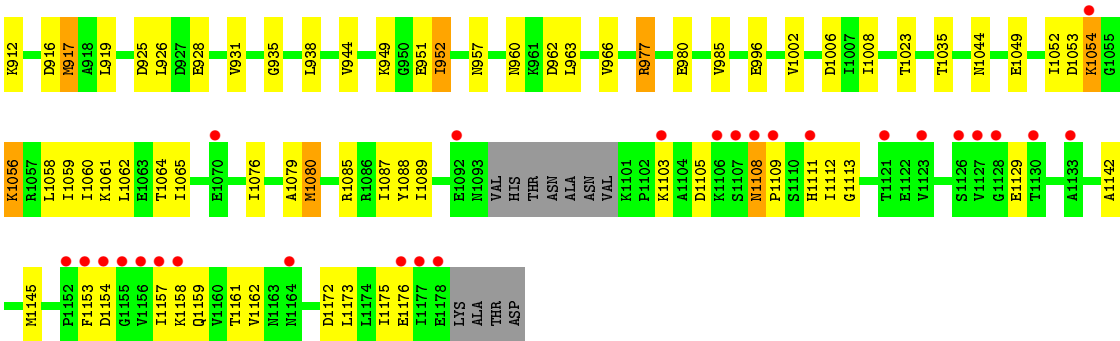






• Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.53Å 257.15Å 130.32Å 90.00° 114.35° 90.00°	Depositor
Resolution (Å)	29.95 – 2.71 29.72 – 2.71	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.95-2.71) 86.2 (29.72-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.279 0.222 , 0.271	Depositor DCC
R_{free} test set	6798 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 135012 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34327	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: MN, BTI, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/9091	0.58	0/12299
1	B	0.37	0/8623	0.53	0/11672
1	C	0.37	0/8601	0.53	1/11624 (0.0%)
1	D	0.40	0/8569	0.55	0/11595
All	All	0.39	0/34884	0.55	1/47190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	494	LEU	CA-CB-CG	5.01	126.82	115.30

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	8923	0	8850	160	0
1	B	8463	0	8410	159	0
1	C	8439	0	8348	142	0
1	D	8411	0	8360	171	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	15	1	0
2	D	15	0	15	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	27	0	12	1	0
All	All	34327	0	34040	622	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 9.

All (622) 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:B:908:ALA:HB1	1:B:909:PRO:HD2	1.35	1.09
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.24	1.01
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.26	1.00
1:B:44:ASN:HD22	1:B:45:ARG:H	1.03	0.98
1:C:504:ILE:HG21	1:C:1042:MET:HE2	1.46	0.96
1:D:44:ASN:HD22	1:D:45:ARG:H	1.12	0.92
1:B:826:THR:HG21	1:B:831:MET:HE2	1.53	0.90
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.35	0.90
1:A:278:ALA:HB1	1:A:279:PRO:HD2	1.55	0.88
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.38	0.88
1:A:44:ASN:HD22	1:A:45:ARG:H	1.21	0.88
1:C:44:ASN:HD22	1:C:45:ARG:H	1.16	0.87
1:D:259:HIS:H	1:D:364:GLN:HE22	1.22	0.85
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.06	0.85
1:A:278:ALA:CB	1:A:279:PRO:HD2	2.07	0.84
1:A:278:ALA:HB1	1:A:279:PRO:CD	2.07	0.84
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.41	0.83
1:D:101:ARG:HH21	1:D:101:ARG:HG2	1.43	0.83
1:D:700:SER:H	1:D:736:HIS:HD2	1.28	0.82
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.62	0.81
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.60	0.81
1:B:700:SER:H	1:B:736:HIS:HD2	1.29	0.81
1:A:700:SER:H	1:A:736:HIS:HD2	1.27	0.81
1:C:54:ARG:CG	1:C:54:ARG:HH11	1.93	0.80
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.30	0.79
1:D:960:ASN:HD22	1:D:963:LEU:H	1.29	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:CG	1:B:77:ARG:HH11	1.99	0.76
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.49	0.76
1:A:504:ILE:HD13	1:A:1042:MET:HE2	1.68	0.76
1:A:896:ARG:HD2	1:A:928:GLU:OE2	1.86	0.76
1:B:48:ILE:O	1:B:52:ILE:HG12	1.86	0.76
1:A:406:ARG:HD3	1:C:403:PHE:HA	1.67	0.76
1:B:44:ASN:ND2	1:B:45:ARG:H	1.83	0.75
1:C:700:SER:H	1:C:736:HIS:HD2	1.33	0.75
1:A:504:ILE:HG21	1:A:1042:MET:HE2	1.70	0.74
1:A:641:MET:HE2	1:A:671:ILE:HG13	1.70	0.73
1:D:1108:ASN:HB2	1:D:1109:PRO:HD3	1.70	0.73
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.72	0.72
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.20	0.72
1:A:363:GLN:HE21	1:A:364:GLN:H	1.39	0.71
1:A:313:LEU:HD13	1:A:323:ILE:HG13	1.72	0.71
1:B:908:ALA:O	1:B:910:SER:N	2.24	0.71
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.25	0.71
1:A:1000:GLY:H	1:A:1001:PRO:HD2	1.55	0.71
1:D:570:PHE:O	1:D:574:HIS:HE1	1.74	0.71
1:D:313:LEU:HB2	1:D:323:ILE:HD11	1.71	0.71
1:B:908:ALA:CB	1:B:909:PRO:HD2	2.15	0.71
1:A:1093:ASN:HB2	1:A:1095:HIS:O	1.92	0.70
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.02	0.70
1:C:116:PRO:HB2	1:C:122:SER:HA	1.74	0.70
1:C:700:SER:H	1:C:736:HIS:CD2	2.08	0.70
1:C:54:ARG:HG2	1:C:54:ARG:HH11	1.56	0.69
1:C:152:LYS:HG3	1:C:197:SER:H	1.55	0.69
1:D:840:THR:O	1:D:843:THR:HB	1.91	0.69
1:B:39:LYS:HB3	1:B:62:SER:HB3	1.75	0.69
1:A:840:THR:O	1:A:843:THR:HB	1.92	0.69
1:B:675:ARG:HA	1:B:701:GLU:HB3	1.75	0.69
1:B:504:ILE:HG21	1:B:1042:MET:CE	2.22	0.69
1:A:278:ALA:CB	1:A:279:PRO:CD	2.68	0.68
1:A:99:ILE:HG23	1:A:127:PHE:HD1	1.58	0.68
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.28	0.68
1:D:142:HIS:H	1:D:145:HIS:HD2	1.43	0.67
1:C:437:LYS:HD3	1:C:437:LYS:H	1.57	0.67
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.10	0.67
1:B:506:ASN:ND2	1:B:510:ASN:HD22	1.93	0.67
1:C:811:ASN:H	1:C:811:ASN:HD22	1.42	0.67
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:927:ASP:H	1:B:930:SER:HB3	1.59	0.66
1:D:350:LEU:HD22	1:D:359:GLU:HB3	1.77	0.66
1:D:101:ARG:HH21	1:D:101:ARG:CG	2.09	0.66
1:A:1064:THR:HG21	1:C:1066:SER:HA	1.76	0.66
1:B:811:ASN:H	1:B:811:ASN:HD22	1.43	0.66
1:B:435:SER:HB3	1:B:438:GLN:HB2	1.78	0.66
1:C:269:ARG:HG3	1:C:270:ARG:H	1.59	0.66
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.78	0.66
1:D:558:LYS:HD2	1:D:765:ASP:O	1.96	0.66
1:A:209:GLU:HG2	1:A:210:GLU:N	2.11	0.65
1:D:470:LYS:HB2	1:D:480:PHE:HE1	1.61	0.65
1:B:750:LYS:HG3	1:C:819:GLY:HA3	1.76	0.65
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.32	0.65
1:A:1081:ASN:HB2	1:C:78:TYR:CE2	2.32	0.65
1:A:209:GLU:CG	1:A:210:GLU:H	2.09	0.64
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.62	0.64
1:A:799:ALA:H	1:A:811:ASN:ND2	1.96	0.64
1:A:209:GLU:CG	1:A:210:GLU:N	2.60	0.64
1:C:51:ARG:NH2	1:C:337:GLU:OE2	2.31	0.64
1:A:328:ARG:HD2	1:A:329:VAL:O	1.98	0.64
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.79	0.63
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.32	0.63
1:D:87:GLY:HA3	1:D:90:LEU:HD12	1.80	0.63
1:C:90:LEU:HB3	1:C:95:SER:HB3	1.79	0.63
1:C:313:LEU:HB2	1:C:323:ILE:HD11	1.81	0.63
1:D:543:GLN:HE22	1:D:636:ASN:HA	1.64	0.63
1:C:54:ARG:NH1	1:C:54:ARG:HG2	2.13	0.62
1:A:143:LEU:HD12	1:A:143:LEU:H	1.64	0.62
1:A:715:ARG:HH12	1:A:865:GLU:CD	2.02	0.62
1:A:641:MET:CE	1:A:671:ILE:HG13	2.28	0.62
1:C:866:MET:CE	1:C:871:TYR:HA	2.29	0.62
1:D:259:HIS:H	1:D:364:GLN:NE2	1.96	0.61
1:A:144:GLU:O	1:A:148:MET:HB2	2.00	0.61
1:C:435:SER:HB2	1:C:437:LYS:HE3	1.82	0.61
1:D:893:MET:O	1:D:897:VAL:HG23	2.00	0.61
1:A:811:ASN:HD22	1:A:811:ASN:H	1.48	0.61
1:B:1057:ARG:HD3	1:B:1059:ILE:HD11	1.82	0.61
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.82	0.61
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.83	0.61
1:D:400:SER:OG	1:D:449:GLU:HB3	2.00	0.61
1:B:864:HIS:HD2	1:B:866:MET:H	1.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:HG2	1:A:320:PHE:HE1	1.64	0.61
1:B:288:ARG:NH1	1:B:288:ARG:HG3	2.01	0.61
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.66	0.61
1:B:504:ILE:HG21	1:B:1042:MET:HE2	1.80	0.61
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.36	0.61
1:D:647:ASN:HD22	1:D:647:ASN:C	2.03	0.60
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.34	0.60
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.31	0.60
1:A:504:ILE:HD13	1:A:1042:MET:CE	2.30	0.60
1:C:269:ARG:HG3	1:C:270:ARG:N	2.16	0.60
1:C:866:MET:HE1	1:C:871:TYR:HA	1.83	0.60
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.31	0.60
1:B:41:LEU:O	1:B:64:VAL:O	2.20	0.60
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.36	0.60
1:B:504:ILE:HD13	1:B:1042:MET:CE	2.31	0.60
1:B:142:HIS:H	1:B:145:HIS:HD2	1.50	0.60
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.84	0.60
1:C:858:ASN:O	1:C:861:ILE:HG12	2.02	0.60
1:D:357:LEU:HA	1:D:360:ILE:HD13	1.83	0.60
1:C:768:ILE:HG22	1:C:791:VAL:HG23	1.83	0.60
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.31	0.60
1:B:927:ASP:HB3	1:B:930:SER:H	1.67	0.59
1:D:1065:ILE:HG12	1:D:1076:ILE:HG12	1.84	0.59
1:A:575:GLN:NE2	1:A:610:ALA:H	2.00	0.59
1:B:934:ASP:O	1:B:938:LEU:HG	2.02	0.59
1:B:1177:ILE:H	1:B:1177:ILE:HD13	1.67	0.59
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.84	0.59
1:A:524:TYR:CD2	1:A:843:THR:HG22	2.36	0.59
1:B:408:ASP:HB2	1:B:428:LYS:HB3	1.84	0.59
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.16	0.59
1:A:700:SER:H	1:A:736:HIS:CD2	2.15	0.59
1:A:814:TYR:CZ	1:A:828:ILE:HG12	2.38	0.59
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.85	0.58
1:A:264:ASP:HB2	1:A:280:SER:HB3	1.84	0.58
1:D:572:ASP:HB3	1:D:807:GLN:HE22	1.66	0.58
1:A:991:ARG:NH2	1:A:1004:GLU:OE1	2.35	0.58
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.84	0.58
1:B:99:ILE:HG23	1:B:127:PHE:HD1	1.68	0.58
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.85	0.58
1:B:41:LEU:HB2	1:B:111:VAL:HG11	1.85	0.58
1:A:1081:ASN:HB2	1:C:78:TYR:CD2	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASP:HB3	1:D:154:LYS:HG3	1.85	0.58
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.68	0.58
1:D:811:ASN:HD22	1:D:811:ASN:H	1.49	0.58
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.86	0.58
1:C:278:ALA:HB3	1:C:335:ILE:HG23	1.86	0.58
1:D:960:ASN:ND2	1:D:963:LEU:H	2.00	0.57
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.85	0.57
1:B:42:VAL:HA	1:B:115:HIS:O	2.05	0.57
1:C:920:TYR:OH	1:C:938:LEU:HB3	2.04	0.57
1:D:1103:LYS:O	1:D:1173:LEU:HB2	2.05	0.57
1:C:41:LEU:HD11	1:C:66:ILE:HG23	1.86	0.56
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.86	0.56
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.56
1:D:1049:GLU:HG2	1:D:1059:ILE:HD12	1.86	0.56
1:B:622:ASN:HD21	1:B:624:TRP:HD1	1.53	0.56
1:A:306:ASN:OD1	1:A:348:GLN:HG2	2.06	0.56
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.70	0.56
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.39	0.56
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.87	0.56
1:D:645:ALA:HB1	1:D:685:GLN:O	2.04	0.56
1:B:1157:ILE:HA	1:B:1177:ILE:HG22	1.86	0.56
1:A:370:LEU:O	1:A:432:HIS:HE1	1.87	0.56
1:D:1061:LYS:HB3	1:D:1079:ALA:HB3	1.87	0.56
1:C:787:ILE:HA	1:C:791:VAL:HG12	1.87	0.56
1:B:377:ARG:HG2	1:B:377:ARG:NH1	2.15	0.56
1:D:935:GLY:HA2	1:D:938:LEU:HD12	1.88	0.56
1:A:145:HIS:HE1	1:A:302:ILE:O	1.87	0.56
1:B:506:ASN:HD22	1:B:510:ASN:HD22	1.53	0.56
1:D:529:ILE:HD13	1:D:589:ASN:HB3	1.88	0.56
1:D:1112:ILE:HD12	1:D:1175:ILE:HB	1.88	0.55
1:D:583:ARG:HD3	1:D:1035:THR:HG23	1.87	0.55
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.88	0.55
1:A:864:HIS:HD2	1:A:866:MET:H	1.54	0.55
1:C:606:MET:HE1	1:C:639:PHE:HB3	1.87	0.55
1:C:225:GLU:HB2	1:C:231:SER:HB3	1.89	0.55
1:A:335:ILE:HD11	1:A:375:GLN:HB3	1.89	0.55
1:D:1142:ALA:HB3	1:D:1145:MET:HB3	1.87	0.55
1:D:866:MET:CE	1:D:871:TYR:HA	2.36	0.55
1:B:370:LEU:O	1:B:432:HIS:HE1	1.89	0.55
1:C:528:SER:O	1:C:530:PRO:HD3	2.07	0.55
1:D:90:LEU:HD13	1:D:95:SER:HA	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:THR:HG21	1:B:330:GLN:HE21	1.72	0.55
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.88	0.55
1:D:864:HIS:HD2	1:D:866:MET:H	1.54	0.55
1:D:866:MET:HE2	1:D:871:TYR:HA	1.90	0.54
1:A:860:GLU:HA	1:A:863:GLN:HE21	1.71	0.54
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.88	0.54
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.71	0.54
1:C:188:GLY:HA3	1:C:237:ARG:HH12	1.71	0.54
1:B:1097:ASN:HB2	1:B:1166:ASP:HA	1.89	0.54
1:A:810:ALA:HB1	1:A:831:MET:CE	2.37	0.54
1:D:1053:ASP:OD2	1:D:1054:LYS:N	2.41	0.54
1:A:58:GLU:HG3	1:C:445:ARG:HD3	1.90	0.54
1:A:278:ALA:O	1:A:279:PRO:C	2.44	0.54
1:A:893:MET:O	1:A:897:VAL:HG23	2.07	0.54
1:D:575:GLN:NE2	1:D:610:ALA:H	2.05	0.54
1:D:1159:GLN:HG2	1:D:1176:GLU:HG2	1.89	0.54
1:B:398:ARG:HG2	1:B:1083:GLN:HE22	1.73	0.54
1:C:53:PHE:CZ	1:C:65:ALA:HB2	2.43	0.54
1:B:606:MET:HE1	1:B:671:ILE:HD13	1.90	0.54
1:C:266:SER:O	1:C:478:THR:HA	2.08	0.54
1:B:504:ILE:HG21	1:B:1042:MET:HE3	1.88	0.54
1:C:717(A):ILE:HG12	1:C:957:ASN:HD21	1.73	0.53
1:C:575:GLN:HE22	1:C:610:ALA:H	1.55	0.53
1:A:44:ASN:ND2	1:A:45:ARG:H	1.99	0.53
1:D:1053:ASP:HB3	1:D:1056:LYS:HG2	1.90	0.53
1:C:39:LYS:HG2	1:C:62:SER:HB3	1.89	0.53
1:A:338:MET:HE3	1:A:373:ALA:HB1	1.91	0.53
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.18	0.53
1:C:167:ILE:HD11	1:C:323:ILE:HD13	1.91	0.53
1:D:846:SER:HA	1:D:849:GLU:HG2	1.90	0.53
1:C:396:ALA:HB3	1:C:453:ARG:HH12	1.73	0.53
1:B:999:GLN:HG2	1:B:1001:PRO:HD3	1.91	0.53
1:C:898:ASN:ND2	1:C:906:LYS:HE3	2.24	0.53
1:D:977:ARG:HG3	1:D:980:GLU:HG3	1.91	0.53
1:B:1053:ASP:HB3	1:B:1056:LYS:HG3	1.90	0.53
1:D:952:ILE:O	1:D:952:ILE:CG2	2.56	0.53
1:D:917:MET:HG2	1:D:944:VAL:HG11	1.90	0.53
1:B:375:GLN:HG3	1:B:430:SER:HB3	1.89	0.53
1:A:446:SER:O	1:A:450:MET:HG2	2.09	0.53
1:A:47:GLU:HB2	1:A:408:ASP:HB3	1.91	0.52
1:A:278:ALA:HB3	1:A:279:PRO:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASN:HD22	1:B:45:ARG:N	1.87	0.52
1:D:44:ASN:ND2	1:D:45:ARG:H	1.94	0.52
1:A:524:TYR:HD2	1:A:843:THR:CG2	2.22	0.52
1:B:435:SER:HB3	1:B:438:GLN:CB	2.39	0.52
1:D:391:THR:HG21	1:D:420:PRO:HG3	1.91	0.52
1:B:341:GLY:O	1:D:434:ILE:HG12	2.09	0.52
1:B:543:GLN:O	1:B:547:GLU:HG2	2.09	0.52
1:B:259:HIS:HB3	1:B:296:ILE:HD11	1.91	0.52
1:C:811:ASN:H	1:C:811:ASN:ND2	2.08	0.52
1:C:71:ASP:C	1:C:73:SER:H	2.11	0.52
1:D:772:THR:HG22	1:D:783:TYR:CE2	2.45	0.52
1:C:209:GLU:HG2	1:C:210:GLU:H	1.75	0.52
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.45	0.52
1:C:948:PHE:HD2	1:C:964:GLN:HG3	1.75	0.52
1:D:575:GLN:HE22	1:D:610:ALA:H	1.57	0.52
1:D:257:ILE:HD12	1:D:300:GLU:HG3	1.92	0.52
1:D:1002:VAL:HG13	1:D:1006:ASP:HB2	1.92	0.52
1:B:905:VAL:HG12	1:B:907:VAL:HG23	1.91	0.52
1:B:574:HIS:HD2	1:B:580:THR:HA	1.75	0.52
1:D:717(A):ILE:HG13	1:D:957:ASN:HD21	1.75	0.52
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.08	0.52
1:D:446:SER:O	1:D:450:MET:HG2	2.10	0.52
1:C:929:GLN:HG2	1:C:932:ILE:HD12	1.92	0.52
1:D:647:ASN:ND2	1:D:647:ASN:C	2.63	0.51
1:A:44:ASN:HD22	1:A:45:ARG:N	1.99	0.51
1:A:641:MET:HG2	1:A:671:ILE:HG21	1.91	0.51
1:C:409:ALA:HA	1:C:427:VAL:HG12	1.92	0.51
1:C:574:HIS:HD2	1:C:580:THR:HA	1.76	0.51
1:C:194:LYS:HB2	1:C:204:MET:HG2	1.92	0.51
1:A:622:ASN:ND2	1:A:624:TRP:H	2.08	0.51
1:C:884:GLY:O	1:C:885:GLU:HB3	2.11	0.51
1:A:266:SER:O	1:A:478:THR:HA	2.10	0.51
1:A:402:GLY:HA3	1:C:54:ARG:HE	1.76	0.51
1:C:1068:PRO:HG3	1:C:1074:ARG:HH11	1.76	0.51
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.45	0.51
1:B:41:LEU:O	1:B:42:VAL:HB	2.11	0.51
1:D:869:GLY:O	1:D:871:TYR:N	2.44	0.51
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.92	0.51
1:A:856:SER:OG	1:D:800:SER:HA	2.11	0.51
1:D:798:VAL:CG1	1:D:835:SER:HA	2.40	0.51
1:C:362:MET:HE3	1:C:362(A):PRO:HD2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:913:VAL:HG22	1:C:943:SER:HB2	1.93	0.50
1:D:756:ILE:HD11	1:D:770:LEU:HD22	1.93	0.50
1:D:254:HIS:NE2	1:D:354:GLY:O	2.45	0.50
1:A:665:GLU:OE1	1:A:668:LYS:HE3	2.12	0.50
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.93	0.50
1:B:404:GLY:O	1:B:431:THR:HA	2.11	0.50
1:A:524:TYR:CD2	1:A:843:THR:CG2	2.95	0.50
1:D:470:LYS:HB2	1:D:480:PHE:CE1	2.44	0.50
1:B:90:LEU:HG	1:B:94:GLU:HB2	1.93	0.50
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.44	0.50
1:D:879:LYS:HG3	1:D:884:GLY:HA3	1.94	0.50
1:B:811:ASN:HD22	1:B:811:ASN:N	2.09	0.50
1:C:1049:GLU:HG2	1:C:1059:ILE:HD12	1.93	0.50
1:C:257:ILE:HD13	1:C:300:GLU:HG3	1.94	0.50
1:B:1153:PHE:CE1	1:B:1177:ILE:HG12	2.46	0.50
1:B:570:PHE:O	1:B:574:HIS:HE1	1.94	0.50
1:C:574:HIS:CD2	1:C:580:THR:HA	2.47	0.50
1:B:755:LEU:O	1:B:759:LEU:HG	2.12	0.50
1:D:38:LYS:HE2	1:D:38:LYS:HA	1.92	0.50
1:C:396:ALA:HB3	1:C:453:ARG:NH1	2.26	0.50
1:C:707:THR:HG22	1:C:708:GLY:H	1.77	0.50
1:D:370:LEU:O	1:D:432:HIS:HE1	1.95	0.50
1:B:574:HIS:CD2	1:B:580:THR:HA	2.46	0.49
1:A:1093:ASN:H	1:A:1093:ASN:ND2	2.10	0.49
1:A:810:ALA:HB1	1:A:831:MET:HE1	1.93	0.49
1:A:519:ARG:HH22	1:A:847:ASP:CG	2.14	0.49
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.59	0.49
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.92	0.49
1:D:641:MET:HE3	1:D:671:ILE:HG21	1.94	0.49
1:C:580:THR:HB	1:C:614:VAL:HG21	1.95	0.49
1:C:223:GLU:O	1:C:227:SER:HB2	2.11	0.49
1:D:574:HIS:CD2	1:D:580:THR:HA	2.47	0.49
1:D:1129:GLU:HB3	1:D:1157:ILE:HD12	1.93	0.49
1:A:191:LEU:HD23	1:A:237:ARG:HA	1.93	0.49
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.95	0.49
1:B:382:ASP:HB3	1:B:456:LYS:O	2.13	0.49
1:A:142:HIS:H	1:A:145:HIS:HD2	1.60	0.49
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.48	0.49
1:A:1120:VAL:HG23	1:A:1166:ASP:O	2.13	0.49
1:C:54:ARG:HG3	1:C:54:ARG:HH11	1.75	0.48
1:B:858:ASN:HD21	1:B:860:GLU:CG	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:HG2	1:A:320:PHE:CE1	2.47	0.48
1:C:419:SER:HB2	1:C:421:TYR:HD1	1.78	0.48
1:A:1000:GLY:N	1:A:1001:PRO:HD2	2.26	0.48
1:C:451:ARG:HG3	1:C:453:ARG:HH21	1.79	0.48
1:D:101:ARG:CG	1:D:101:ARG:NH2	2.73	0.48
1:D:811:ASN:H	1:D:811:ASN:ND2	2.11	0.48
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.95	0.48
1:A:571:ARG:HD3	1:A:605:GLU:OE1	2.12	0.48
1:B:826:THR:HG22	1:B:827:ASP:N	2.28	0.48
1:D:1158:LYS:HB2	1:D:1176:GLU:HG3	1.94	0.48
1:D:259:HIS:HD2	1:D:296:ILE:HD12	1.78	0.48
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.95	0.48
1:C:551:LYS:O	1:C:555:GLU:HG2	2.14	0.48
1:A:278:ALA:O	1:A:280:SER:N	2.47	0.48
1:C:550:PRO:HB2	1:C:736:HIS:CE1	2.48	0.48
1:C:913:VAL:HG13	1:C:944:VAL:HA	1.95	0.48
1:B:1029:ASN:ND2	1:B:1031:SER:OG	2.46	0.48
1:C:667:ALA:HB1	1:C:698:LYS:HE3	1.95	0.48
1:C:276:GLU:O	1:C:335:ILE:HD11	2.14	0.48
1:C:398:ARG:HH11	1:C:451:ARG:HE	1.62	0.48
1:D:574:HIS:HD2	1:D:580:THR:HA	1.79	0.48
1:B:820:PHE:HB3	1:B:821:PRO:HD2	1.95	0.48
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.69	0.48
1:C:259:HIS:HB3	1:C:296:ILE:HD11	1.95	0.48
1:C:338:MET:CE	1:C:430:SER:HB3	2.44	0.47
1:D:799:ALA:H	1:D:811:ASN:ND2	2.12	0.47
1:B:519:ARG:NH2	1:B:846:SER:OG	2.46	0.47
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.95	0.47
1:B:908:ALA:HB1	1:B:909:PRO:CD	2.25	0.47
1:A:1115:GLN:H	1:A:1115:GLN:NE2	2.12	0.47
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.95	0.47
1:A:812:SER:HB2	1:D:778:ASN:HD21	1.79	0.47
1:D:804:LEU:HD13	1:D:854:ILE:HG22	1.95	0.47
1:C:572:ASP:HB3	1:C:807:GLN:HE22	1.80	0.47
1:C:799:ALA:H	1:C:811:ASN:ND2	2.13	0.47
1:C:77:ARG:HD3	1:C:78:TYR:CE2	2.50	0.47
1:A:631:ARG:NH2	1:A:672:ASP:OD1	2.47	0.47
1:D:1044:ASN:HD22	1:D:1062:LEU:HD22	1.79	0.47
1:B:1024:ARG:HB2	1:B:1024:ARG:HH11	1.79	0.47
1:D:41:LEU:HB2	1:D:111:VAL:HG21	1.96	0.47
1:D:661:LYS:HB3	1:D:1008:ILE:HD13	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:THR:HA	1:B:573:ALA:HB3	1.96	0.47
1:A:826:THR:OG1	1:A:827:ASP:N	2.48	0.47
1:A:409:ALA:HA	1:A:427:VAL:HG13	1.96	0.47
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.94	0.47
1:C:263:ARG:HG2	1:C:278:ALA:HB2	1.96	0.47
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.63	0.47
1:C:494:LEU:HB2	1:C:496:ARG:HH11	1.80	0.47
1:C:644:ARG:O	1:C:645:ALA:C	2.52	0.47
1:D:928:GLU:O	1:D:931:VAL:HG12	2.14	0.47
1:A:384:LEU:HD11	1:A:490:ILE:HD11	1.96	0.47
1:D:715:ARG:HH12	1:D:865:GLU:CD	2.18	0.47
1:B:141:PRO:HB2	1:B:145:HIS:HB2	1.96	0.47
1:D:1087:ILE:HG22	1:D:1088:TYR:N	2.30	0.47
1:D:895:ARG:HE	1:D:899:PHE:HE1	1.61	0.47
1:D:912:LYS:NZ	1:D:916:ASP:OD1	2.48	0.47
1:A:496:ARG:HD2	1:A:1052:ILE:HD13	1.96	0.47
1:D:477:THR:HG23	1:D:479:LYS:H	1.79	0.47
1:B:909:PRO:HB2	1:B:952:ILE:HG12	1.97	0.47
1:B:700:SER:H	1:B:736:HIS:CD2	2.20	0.47
1:A:1093:ASN:H	1:A:1093:ASN:HD22	1.63	0.47
1:D:743:MET:CG	1:D:907:VAL:HG13	2.44	0.47
1:A:596:ASP:O	1:A:599:LYS:HG2	2.15	0.47
1:A:672:ASP:HA	1:A:698:LYS:HD2	1.97	0.47
1:A:460:PRO:HA	1:A:463:ILE:HD12	1.96	0.47
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.25	0.46
1:A:521:LYS:HA	1:A:522:PRO:HD3	1.82	0.46
1:B:537:ILE:HA	1:B:538(B):PHE:CD1	2.50	0.46
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.50	0.46
1:D:566:THR:HB	1:D:795:ASP:OD1	2.16	0.46
1:B:558:LYS:HE3	1:B:767:PRO:HD3	1.96	0.46
1:C:260:LEU:HD21	1:C:362:MET:HE1	1.98	0.46
1:B:251:GLY:O	1:B:306:ASN:N	2.47	0.46
1:A:1120:VAL:HG21	1:A:1162:VAL:HB	1.97	0.46
1:C:960:ASN:HB3	1:C:963:LEU:HB3	1.96	0.46
1:D:622:ASN:ND2	1:D:624:TRP:H	2.13	0.46
1:D:828:ILE:O	1:D:832:GLU:HG2	2.16	0.46
1:A:41:LEU:HD13	1:A:106:ALA:HB2	1.97	0.46
1:B:258:VAL:HG22	1:B:357:LEU:HD11	1.96	0.46
1:D:569:THR:HG23	1:D:801:MET:HG3	1.98	0.46
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.80	0.46
1:C:290:ARG:NH2	1:C:318:ASP:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ARG:HG2	1:B:619:LEU:HD22	1.97	0.46
1:C:44:ASN:ND2	1:C:45:ARG:H	1.98	0.46
1:D:1108:ASN:CB	1:D:1109:PRO:HD3	2.44	0.46
1:A:711:LEU:HD21	1:A:750:LYS:HB3	1.98	0.46
1:A:644:ARG:HG2	1:A:647:ASN:OD1	2.16	0.46
1:D:631:ARG:HD3	1:D:631:ARG:HA	1.72	0.46
1:B:715:ARG:C	1:B:715:ARG:HE	2.19	0.46
1:D:826:THR:HG21	1:D:831:MET:HE1	1.98	0.46
1:C:313:LEU:HD13	1:C:323:ILE:HG13	1.98	0.46
1:B:864:HIS:CD2	1:B:866:MET:H	2.31	0.46
1:B:624:TRP:HB3	1:B:1005:GLN:NE2	2.31	0.45
1:A:436:PHE:O	1:A:440:GLU:HB2	2.15	0.45
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.98	0.45
1:C:931:VAL:HA	1:C:935:GLY:H	1.81	0.45
1:D:398:ARG:HH21	1:D:449:GLU:HG2	1.81	0.45
1:B:244:HIS:CD2	1:B:265:CYS:HB2	2.50	0.45
1:B:1123:VAL:HG12	1:B:1164:ASN:OD1	2.15	0.45
1:A:214:GLU:HG2	1:A:214:GLU:O	2.16	0.45
1:B:1053:ASP:HB3	1:B:1056:LYS:CG	2.45	0.45
1:B:558:LYS:NZ	1:B:765:ASP:HB3	2.32	0.45
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.97	0.45
1:D:145:HIS:CE1	1:D:304:TYR:HA	2.51	0.45
1:B:1177:ILE:N	1:B:1177:ILE:HD13	2.31	0.45
1:A:739:ALA:HA	1:A:769:HIS:O	2.17	0.45
1:A:209:GLU:HG3	1:A:210:GLU:H	1.79	0.45
1:B:641:MET:HE3	1:B:674:PHE:HE1	1.82	0.45
1:B:144:GLU:O	1:B:148:MET:HB2	2.16	0.45
1:B:804:LEU:HD13	1:B:854:ILE:HG22	1.99	0.45
1:A:563:VAL:HG21	1:A:787:ILE:HG12	1.98	0.45
1:A:278:ALA:HB3	1:A:373:ALA:H	1.80	0.45
1:C:575:GLN:NE2	1:C:610:ALA:H	2.14	0.45
1:D:67:TYR:CD1	1:D:77:ARG:HG3	2.52	0.45
1:B:575:GLN:HE22	1:B:610:ALA:H	1.63	0.45
1:C:927:ASP:O	1:C:930:SER:HB2	2.17	0.45
1:D:875:SER:HA	1:D:887:PHE:CE1	2.51	0.45
1:B:796:THR:HB	1:B:810:ALA:HB2	1.99	0.45
1:A:589:ASN:HD22	1:A:589:ASN:HA	1.61	0.45
1:A:799:ALA:H	1:A:811:ASN:HD21	1.63	0.45
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.99	0.45
1:B:51:ARG:HD3	1:B:406:ARG:HH22	1.82	0.45
1:C:606:MET:CE	1:C:639:PHE:HB3	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PRO:HB2	1:B:145:HIS:CB	2.47	0.45
1:A:331:VAL:HG23	1:A:332:GLU:OE2	2.17	0.45
1:C:641:MET:HB3	1:C:671:ILE:HD12	1.99	0.44
1:A:540:GLY:H	1:A:543:GLN:HE21	1.64	0.44
1:C:342:ILE:HG12	1:C:362:MET:CE	2.46	0.44
1:D:858:ASN:HD21	1:D:860:GLU:HB2	1.81	0.44
1:D:263:ARG:HH21	1:D:330:GLN:HE21	1.64	0.44
1:B:413:PHE:HE1	1:B:416:ALA:HB3	1.82	0.44
1:C:749:PRO:HG3	1:C:781:LEU:HB3	2.00	0.44
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.82	0.44
1:B:41:LEU:HB3	1:B:114:ILE:HG12	1.99	0.44
1:D:896:ARG:HD2	1:D:928:GLU:OE1	2.17	0.44
1:C:313:LEU:HD11	4:C:2100:ADP:H2'	2.00	0.44
1:B:858:ASN:HD21	1:B:860:GLU:HG2	1.83	0.44
1:D:116:PRO:HB2	1:D:122:SER:HA	2.00	0.44
1:B:522:PRO:HB2	1:B:523:ASP:H	1.66	0.44
1:A:731:GLU:HG3	1:A:766:LEU:HD13	2.00	0.44
1:A:888:ASP:HA	1:A:891:LYS:HE3	2.00	0.44
1:B:631:ARG:HD3	1:B:631:ARG:HA	1.47	0.44
1:B:391:THR:HG23	1:B:420:PRO:HD3	1.98	0.44
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.50	0.44
1:B:597:VAL:HG22	1:B:830:GLY:HA3	1.99	0.44
1:D:700:SER:H	1:D:736:HIS:CD2	2.19	0.44
1:A:551:LYS:O	1:A:555:GLU:HG2	2.18	0.44
1:C:854:ILE:HG13	1:C:854:ILE:H	1.63	0.44
1:D:641:MET:HB3	1:D:671:ILE:HD12	1.99	0.44
1:A:350:LEU:HD13	1:A:359:GLU:HB3	2.00	0.44
1:B:40:LEU:HD11	1:B:349:ILE:HD12	2.00	0.44
1:C:152:LYS:HG3	1:C:197:SER:N	2.30	0.44
1:A:631:ARG:HG2	1:A:670:GLY:HA3	2.00	0.44
1:B:715:ARG:NH1	1:B:865:GLU:OE2	2.47	0.43
1:A:501:LEU:HD21	1:A:1080:MET:HG3	2.00	0.43
1:A:195:ALA:HA	1:A:233:VAL:HG12	1.99	0.43
1:A:811:ASN:H	1:A:811:ASN:ND2	2.12	0.43
1:C:378:ILE:HB	1:C:427:VAL:HG23	2.00	0.43
1:A:258:VAL:HG21	1:A:362:MET:HE2	2.00	0.43
1:D:739:ALA:HA	1:D:769:HIS:O	2.19	0.43
1:C:918:ALA:O	1:C:922:VAL:HG23	2.19	0.43
1:C:775:THR:HG22	1:C:861:ILE:HG13	2.00	0.43
1:B:357:LEU:O	1:B:362:MET:HB3	2.18	0.43
1:D:752:ALA:HB2	1:D:782:THR:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:CYS:HB2	1:A:462:LEU:HD22	1.99	0.43
1:C:866:MET:HE2	1:C:871:TYR:HA	1.99	0.43
1:C:580:THR:O	1:C:614:VAL:HG11	2.18	0.43
1:A:434:ILE:HG13	1:A:434:ILE:H	1.56	0.43
1:B:907:VAL:HB	1:B:908:ALA:H	1.58	0.43
1:B:506:ASN:ND2	1:B:510:ASN:ND2	2.65	0.43
1:A:647:ASN:O	1:A:649:VAL:N	2.52	0.43
1:C:1090:LYS:HB3	1:C:1090:LYS:HE2	1.77	0.43
1:B:828:ILE:O	1:B:831:MET:HB2	2.19	0.43
1:A:258:VAL:HG21	1:A:362:MET:CE	2.48	0.43
1:B:241:ASN:HB2	1:B:477:THR:HG21	2.01	0.43
1:D:655:PRO:HG3	1:D:985:VAL:HG23	1.99	0.43
1:B:565:LEU:HD23	1:B:824:LEU:HD22	2.00	0.43
1:B:571:ARG:C	1:B:571:ARG:HD2	2.39	0.43
1:D:641:MET:HE3	1:D:674:PHE:CE1	2.53	0.43
1:C:144:GLU:O	1:C:148:MET:HB2	2.19	0.43
1:C:704:ILE:HG21	1:C:723:TYR:HD2	1.84	0.43
1:B:913:VAL:HG22	1:B:943:SER:HB2	2.01	0.43
1:D:655:PRO:CG	1:D:985:VAL:HG23	2.48	0.43
1:C:434:ILE:HG13	1:C:434:ILE:H	1.67	0.43
1:B:631:ARG:NH1	1:B:634:ILE:O	2.52	0.43
1:D:622:ASN:C	1:D:622:ASN:HD22	2.22	0.43
1:B:245:ILE:HD13	1:B:264:ASP:HA	2.00	0.43
1:B:1078:TYR:HB2	1:B:1085:ARG:HB3	2.01	0.43
1:C:960:ASN:CB	1:C:963:LEU:HB3	2.49	0.43
1:B:989:LYS:HA	1:B:992:GLU:HB2	2.01	0.43
1:D:1052:ILE:HD13	1:D:1058:LEU:HB2	2.00	0.43
2:C:2000:BTI:H5	1:D:512:PHE:CZ	2.54	0.43
1:B:765:ASP:O	1:B:766:LEU:C	2.57	0.42
1:D:501:LEU:CD1	1:D:1085:ARG:HG2	2.49	0.42
1:C:584:THR:O	1:C:588:ILE:HG12	2.19	0.42
1:C:142:HIS:H	1:C:145:HIS:HD2	1.67	0.42
1:A:42:VAL:HG11	1:A:49:ALA:HA	2.01	0.42
1:D:338:MET:HE1	1:D:430:SER:HB2	2.01	0.42
1:B:1027:TYR:HB3	1:B:1030:LEU:HD21	2.00	0.42
1:D:326:ASN:HA	1:D:327:PRO:HD3	1.91	0.42
1:A:656:ASP:OD1	1:A:688:VAL:HG21	2.19	0.42
1:B:828:ILE:HG13	1:B:828:ILE:H	1.37	0.42
1:A:406:ARG:HA	1:A:406:ARG:NE	2.34	0.42
1:B:558:LYS:HG3	1:B:767:PRO:HG3	2.01	0.42
1:D:1113:GLY:HA2	1:D:1172:ASP:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HB2	1:A:323:ILE:HD11	2.02	0.42
1:B:39:LYS:HD2	1:B:109:ALA:O	2.19	0.42
1:D:1153:PHE:HB3	1:D:1154:ASP:H	1.60	0.42
1:C:382:ASP:HA	1:C:383:PRO:HD3	1.86	0.42
1:D:641:MET:HG2	1:D:671:ILE:HG21	2.01	0.42
1:A:1060:ILE:HG12	1:A:1080:MET:HG2	2.02	0.42
1:C:937:LYS:HG3	1:C:937:LYS:H	1.64	0.42
1:C:917:MET:SD	1:C:944:VAL:HG21	2.60	0.42
1:D:879:LYS:C	1:D:881:LEU:H	2.22	0.42
1:A:1050:ILE:HD12	1:A:1060:ILE:HD12	2.02	0.42
1:B:379:THR:HG22	1:B:425:LEU:HA	2.02	0.42
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.51	0.42
1:B:69:ASN:HD22	1:B:69:ASN:HA	1.67	0.42
1:C:302:ILE:H	1:C:302:ILE:HG13	1.77	0.42
1:C:606:MET:HE3	1:C:607:TRP:HB2	2.01	0.42
1:A:796:THR:HB	1:A:810:ALA:HB2	2.02	0.42
1:B:391:THR:HB	1:B:392:GLY:H	1.65	0.42
1:B:787:ILE:HD13	1:B:817:LEU:HD11	2.01	0.42
1:D:737:ILE:HG12	1:D:767:PRO:HG2	2.01	0.42
1:A:935:GLY:HA3	1:A:966:VAL:HG13	2.01	0.42
1:B:1097:ASN:C	1:B:1099:ASN:H	2.23	0.42
1:A:41:LEU:HB3	1:A:114:ILE:HG12	2.02	0.42
1:D:77:ARG:HD3	1:D:78:TYR:CE2	2.55	0.42
1:D:92:PRO:HD2	1:D:94:GLU:HG2	2.02	0.42
1:C:370:LEU:O	1:C:432:HIS:HE1	2.02	0.42
1:D:1060:ILE:HG12	1:D:1080:MET:HG2	2.01	0.42
1:D:712:ASN:HA	1:D:713:PRO:HD2	1.95	0.42
1:C:71:ASP:C	1:C:73:SER:N	2.73	0.42
1:B:870:GLN:HA	1:B:873:ASN:HD22	1.84	0.42
1:A:1151:ALA:HA	1:A:1152:PRO:HD3	1.89	0.42
1:C:408:ASP:HB2	1:C:428:LYS:HB3	2.01	0.42
1:D:622:ASN:HD22	1:D:623:PRO:N	2.18	0.41
1:A:773:HIS:ND1	1:A:805:THR:O	2.39	0.41
1:B:436:PHE:O	1:B:440:GLU:HB2	2.19	0.41
1:B:39:LYS:HG3	1:B:111:VAL:HA	2.02	0.41
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.85	0.41
1:C:606:MET:HE1	1:C:671:ILE:HD13	2.01	0.41
1:A:828:ILE:HG13	1:A:828:ILE:H	1.60	0.41
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	2.01	0.41
1:A:622:ASN:HD21	1:A:624:TRP:HD1	1.68	0.41
1:C:972:GLU:HB2	1:C:973:ALA:H	1.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ILE:HG13	1:B:434:ILE:H	1.67	0.41
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.23	0.41
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.15	0.41
1:A:364:GLN:HA	1:A:367:ILE:HD12	2.02	0.41
1:B:934:ASP:HB2	1:B:937:LYS:HE2	2.03	0.41
1:B:309:THR:HG21	1:B:330:GLN:NE2	2.34	0.41
1:D:263:ARG:HG2	1:D:278:ALA:HB2	2.01	0.41
1:D:1105:ASP:HB3	1:D:1111:HIS:ND1	2.35	0.41
1:C:968:LEU:O	1:C:969:LYS:C	2.58	0.41
1:D:570:PHE:O	1:D:574:HIS:CE1	2.62	0.41
1:C:338:MET:HE2	1:C:430:SER:HB3	2.03	0.41
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.34	0.41
1:D:582:VAL:HA	1:D:845:TYR:CZ	2.56	0.41
1:A:89:ASP:HB2	1:A:101:ARG:HH12	1.84	0.41
1:A:818:ASN:N	1:A:818:ASN:HD22	2.18	0.41
1:B:45:ARG:HD2	1:B:71:ASP:OD2	2.21	0.41
1:C:44:ASN:HD22	1:C:45:ARG:N	1.98	0.41
1:C:334:THR:O	1:C:338:MET:HG3	2.21	0.41
1:B:145:HIS:HE1	1:B:302:ILE:O	2.03	0.41
1:D:951:GLU:O	1:D:952:ILE:HD13	2.20	0.41
1:A:1157:ILE:HG13	1:A:1177:ILE:HG12	2.03	0.41
1:C:274:VAL:HG12	1:C:275:VAL:HG23	2.01	0.41
1:B:349:ILE:HG12	1:B:349:ILE:H	1.73	0.41
1:A:388:MET:HA	1:A:389:PRO:HD3	1.81	0.41
1:B:66:ILE:O	1:B:66:ILE:HG13	2.20	0.41
1:B:137:LYS:HA	1:B:137:LYS:HD2	1.84	0.41
1:D:960:ASN:HD21	1:D:962:ASP:HB2	1.86	0.41
1:D:1076:ILE:HD12	1:D:1089:ILE:HD13	2.03	0.41
1:D:406:ARG:NH2	1:D:408:ASP:OD1	2.53	0.41
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.18	0.41
1:C:406:ARG:NH1	1:C:408:ASP:OD1	2.54	0.41
1:B:977:ARG:NH1	1:B:980:GLU:HB3	2.35	0.41
1:C:252:ASP:HB3	1:C:357:LEU:HD13	2.03	0.41
1:D:382:ASP:HA	1:D:383:PRO:HD2	1.87	0.41
1:C:91:GLY:HA3	1:C:92:PRO:HD3	1.78	0.41
1:C:556:TRP:O	1:C:560:GLN:HG2	2.21	0.41
1:A:524:TYR:CE2	1:A:843:THR:HG22	2.56	0.41
1:D:1087:ILE:CG2	1:D:1088:TYR:N	2.84	0.41
1:A:241:ASN:N	1:A:242:PRO:HD3	2.36	0.41
1:B:647:ASN:O	1:B:649:VAL:N	2.54	0.41
1:D:365:LYS:H	1:D:365:LYS:HG2	1.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:ILE:HB	1:D:460:PRO:HD3	2.03	0.41
1:A:524:TYR:HD2	1:A:843:THR:HG21	1.85	0.40
1:D:263:ARG:HH21	1:D:330:GLN:NE2	2.19	0.40
1:C:230:ASN:HD22	1:C:232:GLU:H	1.68	0.40
1:C:907:VAL:O	1:C:910:SER:N	2.55	0.40
1:D:289:GLN:HA	1:D:289:GLN:HE21	1.85	0.40
1:A:587:MET:O	1:A:590:ILE:HD12	2.21	0.40
1:A:810:ALA:CB	1:A:831:MET:HE3	2.51	0.40
1:C:448:ARG:HH22	1:C:467:LYS:HE3	1.86	0.40
1:B:357(B):GLY:C	1:B:359:GLU:H	2.24	0.40
1:D:755:LEU:O	1:D:759:LEU:HG	2.20	0.40
1:B:394:ILE:HG13	1:B:394:ILE:H	1.76	0.40
1:D:885:GLU:HA	1:D:885:GLU:OE2	2.22	0.40
1:D:820:PHE:HB3	1:D:821:PRO:CD	2.52	0.40
1:D:828:ILE:HG13	1:D:828:ILE:H	1.57	0.40
1:D:494:LEU:HD23	1:D:495:ASP:N	2.37	0.40
1:D:673:VAL:HG22	1:D:699:ILE:HD12	2.03	0.40
1:A:156:ARG:HB3	1:A:156:ARG:HH11	1.86	0.40
1:A:99:ILE:HG23	1:A:127:PHE:CD1	2.45	0.40
1:C:342:ILE:HG12	1:C:362:MET:HE3	2.02	0.40
1:B:1050:ILE:HD12	1:B:1060:ILE:HD12	2.04	0.40
1:B:582:VAL:HA	1:B:845:TYR:CZ	2.56	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	1125/1150 (98%)	1034 (92%)	76 (7%)	15 (1%)	15	36
1	B	1070/1150 (93%)	981 (92%)	75 (7%)	14 (1%)	15	36
1	C	1063/1150 (92%)	968 (91%)	79 (7%)	16 (2%)	13	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1061/1150 (92%)	985 (93%)	70 (7%)	6 (1%)	30	58
All	All	4319/4600 (94%)	3968 (92%)	300 (7%)	51 (1%)	16	38

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	278	ALA
1	A	648	ALA
1	B	909	PRO
1	B	1001	PRO
1	C	92	PRO
1	C	168	PRO
1	D	92	PRO
1	D	870	GLN
1	A	209	GLU
1	A	999	GLN
1	A	1000	GLY
1	B	391	THR
1	B	518	LYS
1	B	522	PRO
1	B	766	LEU
1	B	907	VAL
1	C	87	GLY
1	C	199	GLY
1	C	518	LYS
1	C	645	ALA
1	D	868	GLY
1	A	195	ALA
1	A	213	LEU
1	A	518	LYS
1	A	868	GLY
1	A	1081	ASN
1	B	162	ALA
1	B	648	ALA
1	B	903	ASP
1	C	184	ALA
1	C	189	PHE
1	C	197	SER
1	D	1108	ASN
1	A	210	GLU
1	B	42	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1002	VAL
1	B	1098	ALA
1	C	425	LEU
1	C	885	GLU
1	D	317	GLY
1	D	648	ALA
1	A	1097	ASN
1	C	648	ALA
1	A	1094	VAL
1	C	91	GLY
1	B	87	GLY
1	C	190	PRO
1	C	1014	PRO
1	A	434	ILE
1	C	1001	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	974/986 (99%)	893 (92%)	81 (8%)	14	31
1	B	927/986 (94%)	867 (94%)	60 (6%)	21	45
1	C	916/986 (93%)	833 (91%)	83 (9%)	12	26
1	D	921/986 (93%)	860 (93%)	61 (7%)	21	44
All	All	3738/3944 (95%)	3453 (92%)	285 (8%)	16	36

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	60	ASP
1	A	62	SER
1	A	69	ASN
1	A	108	GLN
1	A	122	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	GLU
1	A	156	ARG
1	A	166	VAL
1	A	167	ILE
1	A	181	LYS
1	A	189	PHE
1	A	207	VAL
1	A	209	GLU
1	A	210	GLU
1	A	213	LEU
1	A	214	GLU
1	A	241	ASN
1	A	271	HIS
1	A	287	LEU
1	A	306	ASN
1	A	329	VAL
1	A	331	VAL
1	A	368	THR
1	A	417	GLU
1	A	423	ASP
1	A	427	VAL
1	A	455	VAL
1	A	473	SER
1	A	506	ASN
1	A	519	ARG
1	A	525	GLU
1	A	526	LEU
1	A	542	LYS
1	A	571	ARG
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	606	MET
1	A	607	TRP
1	A	622	ASN
1	A	631	ARG
1	A	707	THR
1	A	715	ARG
1	A	743	MET
1	A	750	LYS
1	A	761	SER
1	A	766	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	772	THR
1	A	775	THR
1	A	812	SER
1	A	828	ILE
1	A	855	LYS
1	A	856	SER
1	A	861	ILE
1	A	863	GLN
1	A	871	TYR
1	A	907	VAL
1	A	919	LEU
1	A	926	LEU
1	A	931	VAL
1	A	944	VAL
1	A	945	VAL
1	A	966	VAL
1	A	980	GLU
1	A	991	ARG
1	A	999	GLN
1	A	1008	ILE
1	A	1029	ASN
1	A	1043	ARG
1	A	1051	GLU
1	A	1064	THR
1	A	1080	MET
1	A	1085	ARG
1	A	1089	ILE
1	A	1090	LYS
1	A	1093	ASN
1	A	1115	GLN
1	A	1116	MET
1	A	1148	THR
1	A	1153	PHE
1	B	40	LEU
1	B	44	ASN
1	B	75	LEU
1	B	77	ARG
1	B	95	SER
1	B	110	ASN
1	B	154	LYS
1	B	156	ARG
1	B	157	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	241	ASN
1	B	249	VAL
1	B	250	ILE
1	B	288	ARG
1	B	306	ASN
1	B	320	PHE
1	B	329	VAL
1	B	357	LEU
1	B	377	ARG
1	B	391	THR
1	B	394	ILE
1	B	403	PHE
1	B	407	LEU
1	B	413	PHE
1	B	417	GLU
1	B	458	ASN
1	B	461	PHE
1	B	496	ARG
1	B	523	ASP
1	B	524	TYR
1	B	528	SER
1	B	580	THR
1	B	588	ILE
1	B	606	MET
1	B	607	TRP
1	B	631	ARG
1	B	649	VAL
1	B	715	ARG
1	B	743	MET
1	B	750	LYS
1	B	781	LEU
1	B	784	LYS
1	B	811	ASN
1	B	828	ILE
1	B	855	LYS
1	B	880	SER
1	B	926	LEU
1	B	952	ILE
1	B	986	ASP
1	B	991	ARG
1	B	996	GLU
1	B	1008	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1024	ARG
1	B	1029	ASN
1	B	1051	GLU
1	B	1085	ARG
1	B	1097	ASN
1	B	1147	THR
1	B	1148	THR
1	B	1175	ILE
1	B	1177	ILE
1	C	44	ASN
1	C	54	ARG
1	C	60	ASP
1	C	86	VAL
1	C	97	LEU
1	C	98	ASN
1	C	112	ASP
1	C	179	LEU
1	C	183	PHE
1	C	185	GLU
1	C	189	PHE
1	C	193	ILE
1	C	196	THR
1	C	227	SER
1	C	230	ASN
1	C	262	GLU
1	C	269	ARG
1	C	287	LEU
1	C	313	LEU
1	C	329	VAL
1	C	335	ILE
1	C	377	ARG
1	C	398	ARG
1	C	406	ARG
1	C	414	GLN
1	C	417	GLU
1	C	427	VAL
1	C	437	LYS
1	C	445	ARG
1	C	451	ARG
1	C	456	LYS
1	C	472	THR
1	C	494	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	515	ASN
1	C	519	ARG
1	C	526	LEU
1	C	535	SER
1	C	542	LYS
1	C	543	GLN
1	C	580	THR
1	C	592	SER
1	C	606	MET
1	C	607	TRP
1	C	617	ASN
1	C	641	MET
1	C	649	VAL
1	C	707	THR
1	C	717	ASN
1	C	719	THR
1	C	743	MET
1	C	780	LEU
1	C	792	ASP
1	C	807	GLN
1	C	811	ASN
1	C	828	ILE
1	C	843	THR
1	C	854	ILE
1	C	855	LYS
1	C	866	MET
1	C	888	ASP
1	C	892	ASP
1	C	906	LYS
1	C	907	VAL
1	C	931	VAL
1	C	936	TYR
1	C	937	LYS
1	C	942	GLU
1	C	959	PHE
1	C	960	ASN
1	C	969	LYS
1	C	971	GLN
1	C	972	GLU
1	C	999	GLN
1	C	1008	ILE
1	C	1022	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	C	1053	ASP
1	C	1054	LYS
1	C	1085	ARG
1	C	1090	LYS
1	C	1147	THR
1	D	44	ASN
1	D	60	ASP
1	D	62	SER
1	D	101	ARG
1	D	122	SER
1	D	239	ILE
1	D	262	GLU
1	D	288	ARG
1	D	289	GLN
1	D	296	ILE
1	D	329	VAL
1	D	335	ILE
1	D	414	GLN
1	D	419	SER
1	D	427	VAL
1	D	434	ILE
1	D	455	VAL
1	D	456	LYS
1	D	523	ASP
1	D	525	GLU
1	D	531	THR
1	D	542	LYS
1	D	580	THR
1	D	588	ILE
1	D	607	TRP
1	D	620	LYS
1	D	622	ASN
1	D	629	ARG
1	D	631	ARG
1	D	632	LYS
1	D	647	ASN
1	D	649	VAL
1	D	707	THR
1	D	715	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	743	MET
1	D	760	LYS
1	D	775	THR
1	D	781	LEU
1	D	807	GLN
1	D	828	ILE
1	D	853	ASP
1	D	855	LYS
1	D	856	SER
1	D	880	SER
1	D	886	ARG
1	D	895	ARG
1	D	907	VAL
1	D	917	MET
1	D	919	LEU
1	D	925	ASP
1	D	926	LEU
1	D	949	LYS
1	D	952	ILE
1	D	977	ARG
1	D	996	GLU
1	D	1054	LYS
1	D	1056	LYS
1	D	1064	THR
1	D	1080	MET
1	D	1161	THR
1	D	1162	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	110	ASN
1	A	145	HIS
1	A	241	ASN
1	A	244	HIS
1	A	254	HIS
1	A	256	ASN
1	A	326	ASN
1	A	330	GLN
1	A	363	GLN
1	A	432	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	617	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	863	GLN
1	A	864	HIS
1	A	873	ASN
1	A	898	ASN
1	A	957	ASN
1	A	1005	GLN
1	A	1019	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	A	1081	ASN
1	A	1093	ASN
1	A	1095	HIS
1	A	1099	ASN
1	A	1108	ASN
1	A	1134	ASN
1	A	1135	GLN
1	B	44	ASN
1	B	69	ASN
1	B	145	HIS
1	B	244	HIS
1	B	330	GLN
1	B	375	GLN
1	B	385	ASN
1	B	432	HIS
1	B	506	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	736	HIS
1	B	778	ASN
1	B	807	GLN
1	B	811	ASN
1	B	858	ASN
1	B	864	HIS
1	B	873	ASN
1	B	877	GLN
1	B	898	ASN
1	B	923	GLN
1	B	971	GLN
1	B	1005	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1083	GLN
1	B	1111	HIS
1	C	44	ASN
1	C	108	GLN
1	C	145	HIS
1	C	230	ASN
1	C	326	ASN
1	C	330	GLN
1	C	385	ASN
1	C	432	HIS
1	C	506	ASN
1	C	574	HIS
1	C	575	GLN
1	C	617	ASN
1	C	622	ASN
1	C	653	ASN
1	C	660	HIS
1	C	685	GLN
1	C	694	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	877	GLN
1	C	898	ASN
1	C	924	ASN
1	C	957	ASN
1	C	971	GLN
1	C	1025	ASN
1	C	1029	ASN
1	D	44	ASN
1	D	145	HIS
1	D	241	ASN
1	D	289	GLN
1	D	301	ASN
1	D	326	ASN
1	D	330	GLN
1	D	364	GLN
1	D	432	HIS
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	622	ASN
1	D	647	ASN
1	D	736	HIS
1	D	778	ASN
1	D	807	GLN
1	D	811	ASN
1	D	818	ASN
1	D	858	ASN
1	D	863	GLN
1	D	864	HIS
1	D	898	ASN
1	D	960	ASN
1	D	1005	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1083	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 ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
2	BTI	A	2000	1	14,16,16	1.85	3 (21%)	13,21,21	1.28	1 (7%)
2	BTI	B	2000	1	14,16,16	1.83	2 (14%)	13,21,21	1.72	3 (23%)
2	BTI	C	2000	1	14,16,16	1.93	4 (28%)	13,21,21	1.44	1 (7%)
4	ADP	C	2100	-	22,29,29	1.08	2 (9%)	27,45,45	1.94	4 (14%)
2	BTI	D	2000	1	14,16,16	1.95	4 (28%)	13,21,21	1.50	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BTI	A	2000	1	-	0/5/27/27	0/2/2/2
2	BTI	B	2000	1	-	0/5/27/27	0/2/2/2
2	BTI	C	2000	1	-	0/5/27/27	0/2/2/2
4	ADP	C	2100	-	-	0/12/32/32	0/3/3/3
2	BTI	D	2000	1	-	0/5/27/27	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	BTI	C2-S1	-3.82	1.76	1.82
2	C	2000	BTI	C2-S1	-3.71	1.76	1.82
2	B	2000	BTI	C2-S1	-3.44	1.77	1.82
2	A	2000	BTI	C2-S1	-3.20	1.77	1.82
2	D	2000	BTI	C3-N3	-2.26	1.32	1.35
2	D	2000	BTI	C3-N2	-2.19	1.32	1.35
2	C	2000	BTI	C3-N2	-2.17	1.32	1.35
2	C	2000	BTI	C3-N3	-2.11	1.32	1.35
2	A	2000	BTI	C3-N2	-2.10	1.32	1.35
4	C	2100	ADP	O4'-C1'	2.24	1.44	1.41
4	C	2100	ADP	C5-C4	3.16	1.47	1.40
2	C	2000	BTI	O3-C3	4.78	1.33	1.23
2	D	2000	BTI	O3-C3	4.83	1.33	1.23
2	B	2000	BTI	O3-C3	4.90	1.33	1.23
2	A	2000	BTI	O3-C3	4.96	1.33	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2100	ADP	N3-C2-N1	-7.23	123.36	128.89
4	C	2100	ADP	C2'-C1'-N9	-3.66	108.70	114.29
4	C	2100	ADP	C4-C5-N7	-3.05	106.67	109.48
4	C	2100	ADP	PA-O3A-PB	-2.90	122.96	132.67
2	B	2000	BTI	O3-C3-N2	-2.08	123.49	125.90
2	B	2000	BTI	C5-N3-C3	-2.01	110.98	112.49
2	A	2000	BTI	N2-C3-N3	3.07	111.00	108.88
2	C	2000	BTI	N2-C3-N3	3.54	111.33	108.88
2	D	2000	BTI	N2-C3-N3	3.75	111.48	108.88
2	B	2000	BTI	N2-C3-N3	4.03	111.67	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	BTI	1	0
4	C	2100	ADP	1	0

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	1131/1150 (98%)	0.10	72 (6%) 23 22	25, 52, 127, 194	0
1	B	1074/1150 (93%)	0.39	82 (7%) 17 15	40, 76, 133, 169	0
1	C	1067/1150 (92%)	0.21	53 (4%) 32 32	43, 70, 103, 140	0
1	D	1067/1150 (92%)	0.13	68 (6%) 23 22	23, 57, 130, 250	0
All	All	4339/4600 (94%)	0.20	275 (6%) 23 23	23, 67, 126, 250	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	TYR	7.6
1	B	1095	HIS	7.0
1	B	397	TYR	6.8
1	C	933	THR	6.4
1	D	1156	VAL	6.2
1	B	380	THR	6.1
1	D	1153	PHE	6.0
1	B	240	ASP	6.0
1	B	398	ARG	5.9
1	A	197	SER	5.8
1	B	415	GLY	5.7
1	B	421	TYR	5.7
1	B	413	PHE	5.7
1	C	932	ILE	5.6
1	A	1156	VAL	5.4
1	D	1178	GLU	5.3
1	A	218	HIS	5.3
1	D	1128	GLY	5.3
1	B	387	PHE	5.2
1	D	271	HIS	5.2
1	B	394	ILE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	393	THR	5.1
1	B	386	ASP	5.1
1	D	168	PRO	5.1
1	A	1137	LEU	5.0
1	B	395	ILE	5.0
1	B	389	PRO	4.9
1	D	1155	GLY	4.9
1	A	1132	LYS	4.9
1	A	1094	VAL	4.9
1	A	177	TYR	4.9
1	D	282	GLY	4.8
1	B	388	MET	4.8
1	B	492	PRO	4.8
1	C	1001	PRO	4.8
1	A	1127	VAL	4.8
1	D	91	GLY	4.8
1	A	1138	LEU	4.7
1	A	206	ILE	4.7
1	B	385	ASN	4.6
1	A	217	PHE	4.6
1	B	384	LEU	4.6
1	A	395	ILE	4.5
1	B	392	GLY	4.5
1	A	494	LEU	4.4
1	B	524	TYR	4.4
1	A	174	ILE	4.4
1	A	195	ALA	4.4
1	B	457	THR	4.4
1	A	1095	HIS	4.3
1	D	153	VAL	4.3
1	D	494	LEU	4.3
1	A	196	THR	4.3
1	A	1001	PRO	4.3
1	A	215	ASP	4.3
1	C	492	PRO	4.2
1	B	402	GLY	4.2
1	A	1128	GLY	4.1
1	A	205	ARG	4.1
1	D	1154	ASP	4.0
1	D	152	LYS	4.0
1	A	219	ARG	3.9
1	B	961	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	526	LEU	3.9
1	B	1096	THR	3.9
1	D	1127	VAL	3.9
1	D	314	VAL	3.9
1	C	1140	THR	3.8
1	B	89	ASP	3.8
1	D	1177	ILE	3.7
1	C	89	ASP	3.7
1	B	938	LEU	3.7
1	A	388	MET	3.7
1	D	1157	ILE	3.7
1	A	90	LEU	3.6
1	D	1107	SER	3.6
1	B	490	ILE	3.6
1	D	1130	THR	3.6
1	D	1126	SER	3.5
1	B	1094	VAL	3.5
1	D	243	LYS	3.5
1	B	153	VAL	3.5
1	B	407	LEU	3.5
1	C	421	TYR	3.5
1	A	188	GLY	3.5
1	D	241	ASN	3.4
1	C	1146	GLU	3.4
1	A	222	SER	3.4
1	B	168	PRO	3.4
1	C	770	LEU	3.4
1	B	93	ALA	3.4
1	D	386	ASP	3.4
1	D	1152	PRO	3.4
1	C	176	SER	3.4
1	C	282	GLY	3.3
1	B	418	ILE	3.3
1	D	309	THR	3.3
1	A	1096	THR	3.3
1	C	1147	THR	3.3
1	D	1123	VAL	3.3
1	B	403	PHE	3.3
1	D	490	ILE	3.3
1	A	207	VAL	3.3
1	B	101	ARG	3.3
1	B	937	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	417	GLU	3.2
1	C	934	ASP	3.2
1	C	494	LEU	3.2
1	A	194	LYS	3.2
1	A	469	LYS	3.2
1	C	970	GLY	3.2
1	C	1093	ASN	3.2
1	C	931	VAL	3.1
1	B	401	GLY	3.1
1	C	972	GLU	3.1
1	A	232	GLU	3.1
1	C	182	GLU	3.1
1	A	1135	GLN	3.1
1	A	175	LYS	3.0
1	D	89	ASP	3.0
1	B	494	LEU	3.0
1	D	151	ASP	3.0
1	A	396	ALA	3.0
1	B	488	PHE	3.0
1	A	453	ARG	3.0
1	D	384	LEU	3.0
1	A	211	SER	3.0
1	C	971	GLN	3.0
1	C	416	ALA	3.0
1	A	1136	PRO	3.0
1	A	176	SER	2.9
1	D	240	ASP	2.9
1	B	981	TYR	2.9
1	B	420	PRO	2.9
1	C	183	PHE	2.9
1	B	88	SER	2.9
1	A	1148	THR	2.9
1	B	412	GLY	2.9
1	D	310	VAL	2.9
1	A	224	ALA	2.9
1	D	156	ARG	2.9
1	B	452	ILE	2.9
1	D	247	VAL	2.9
1	B	527	ALA	2.9
1	A	394	ILE	2.8
1	D	879	LYS	2.8
1	D	417	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	286	THR	2.8
1	C	218	HIS	2.8
1	A	384	LEU	2.8
1	B	271	HIS	2.8
1	D	1158	LYS	2.8
1	B	285	PRO	2.8
1	B	454	GLY	2.8
1	D	283	LEU	2.8
1	A	208	ARG	2.8
1	D	492	PRO	2.8
1	A	1178	GLU	2.7
1	C	993	LEU	2.7
1	A	1130	THR	2.7
1	B	92	PRO	2.7
1	C	215	ASP	2.7
1	D	882	GLY	2.7
1	B	90	LEU	2.7
1	D	1164	ASN	2.7
1	A	386	ASP	2.7
1	C	491	GLN	2.7
1	C	493	SER	2.7
1	C	384	LEU	2.7
1	B	282	GLY	2.7
1	D	388	MET	2.7
1	A	178	GLU	2.7
1	D	1103	LYS	2.6
1	A	1158	LYS	2.6
1	B	119	GLY	2.6
1	C	209	GLU	2.6
1	D	88	SER	2.6
1	D	1106	LYS	2.6
1	D	1176	GLU	2.6
1	A	220	ALA	2.6
1	A	91	GLY	2.6
1	A	221	LYS	2.6
1	D	1109	PRO	2.6
1	B	87	GLY	2.5
1	B	1054	LYS	2.5
1	B	929	GLN	2.5
1	D	1111	HIS	2.5
1	A	398	ARG	2.5
1	B	456	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	391	THR	2.5
1	B	91	GLY	2.5
1	C	185	GLU	2.5
1	B	357(A)	PHE	2.5
1	B	357(B)	GLY	2.4
1	C	687	LYS	2.4
1	B	996	GLU	2.4
1	A	1123	VAL	2.4
1	C	198	GLY	2.4
1	C	199	GLY	2.4
1	D	110	ASN	2.4
1	D	308	GLY	2.4
1	A	420	PRO	2.4
1	C	772	THR	2.4
1	C	208	ARG	2.4
1	C	643	LEU	2.4
1	C	203	GLY	2.4
1	A	88	SER	2.4
1	D	321	PHE	2.3
1	D	421	TYR	2.3
1	B	356	ASP	2.3
1	C	893	MET	2.3
1	B	269	ARG	2.3
1	C	1142	ALA	2.3
1	C	740	ILE	2.3
1	B	396	ALA	2.3
1	C	999	GLN	2.3
1	A	1093	ASN	2.3
1	A	1142	ALA	2.3
1	B	381	GLU	2.3
1	B	641	MET	2.3
1	D	1133	ALA	2.3
1	C	309	THR	2.3
1	C	496	ARG	2.3
1	B	460	PRO	2.3
1	A	223	GLU	2.2
1	A	216	ALA	2.2
1	C	214	GLU	2.2
1	D	1092	GLU	2.2
1	A	89	ASP	2.2
1	B	739	ALA	2.2
1	C	517	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1001	PRO	2.2
1	D	38	LYS	2.2
1	B	270	ARG	2.2
1	B	461	PHE	2.2
1	D	92	PRO	2.2
1	B	377	ARG	2.2
1	D	1121	THR	2.2
1	B	160	ILE	2.2
1	C	490	ILE	2.2
1	A	92	PRO	2.2
1	C	217	PHE	2.2
1	C	110	ASN	2.2
1	D	272	GLN	2.1
1	C	705	CYS	2.1
1	A	193	ILE	2.1
1	D	1108	ASN	2.1
1	D	239	ILE	2.1
1	A	189	PHE	2.1
1	B	422	TYR	2.1
1	D	143	LEU	2.1
1	D	493	SER	2.1
1	D	285	PRO	2.1
1	B	982	LEU	2.1
1	C	648	ALA	2.1
1	A	456	LYS	2.1
1	C	935	GLY	2.1
1	A	1131	VAL	2.1
1	A	1149	ILE	2.1
1	C	175	LYS	2.1
1	B	284	SER	2.1
1	B	263	ARG	2.0
1	B	167	ILE	2.0
1	A	999	GLN	2.0
1	D	248	GLN	2.0
1	B	1097	ASN	2.0
1	D	1054	LYS	2.0
1	A	331	VAL	2.0
1	D	1070	GLU	2.0
1	D	242	PRO	2.0
1	A	239	ILE	2.0
1	C	388	MET	2.0
1	B	410	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1000	GLY	2.0
1	A	487	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
3	MN	C	2002	1/1	0.95	0.37	2.03	103,103,103,103	0
2	BTI	A	2000	15/15	0.92	0.20	0.84	65,67,69,69	0
2	BTI	C	2000	15/15	0.96	0.19	0.49	58,59,70,70	0
3	MN	D	2002	1/1	0.93	0.19	0.20	54,54,54,54	0
3	MN	A	2002	1/1	0.94	0.20	0.14	54,54,54,54	0
2	BTI	B	2000	15/15	0.95	0.15	0.03	50,51,56,57	0
2	BTI	D	2000	15/15	0.93	0.17	-0.32	64,66,67,69	0
3	MN	B	2002	1/1	0.98	0.15	-0.68	75,75,75,75	0
4	ADP	C	2100	27/27	0.93	0.17	-0.75	92,92,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.