



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:49 am GMT

PDB ID : 2C3U
Title : CRYSTAL STRUCTURE OF PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS, OXYGEN INHIBITED FORM
Authors : Cavazza, C.; Contreras-Martel, C.; Pieulle, L.; Chabriere, E.; Hatchikian, E.C.; Fontecilla-Camps, J.C.
Deposited on : 2005-10-12
Resolution : 2.32 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

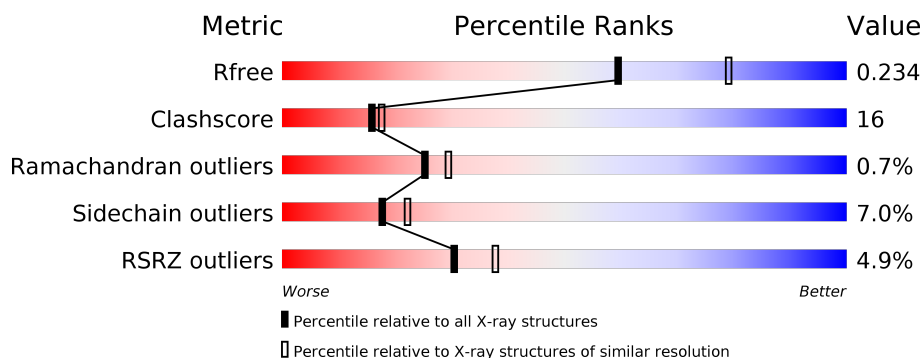
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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	1231	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>
1	B	1231	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19646 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-FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



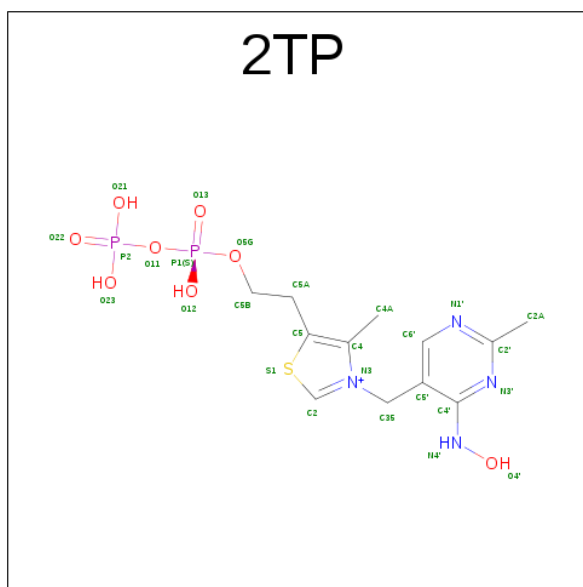
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

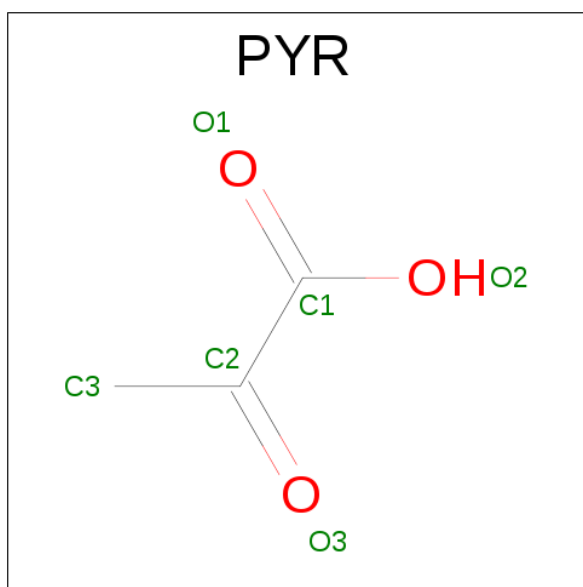
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is 2-(3-{[4-(HYDROXYAMINO)-2-METHYLPYRIMIDIN-5-YL]METHYL}-4-METHYL-2,3-DIHYDRO-1,3-THIAZOL-5-YL)ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: 2TP) (formula: $C_{12}H_{19}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	327	Total	O	0	0
			327	327		

Continued on next page...

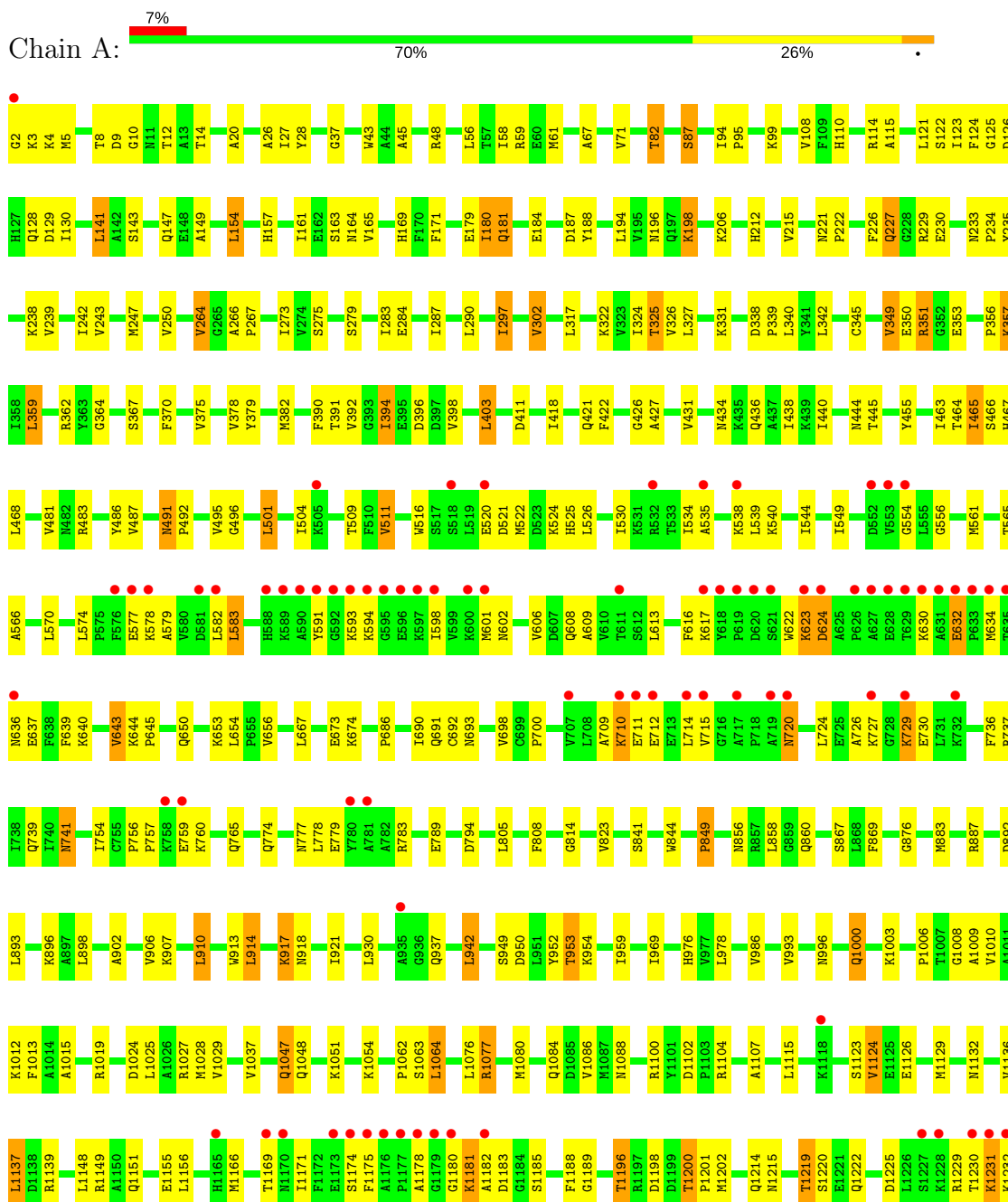
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	435	Total 435	O 435	0	0

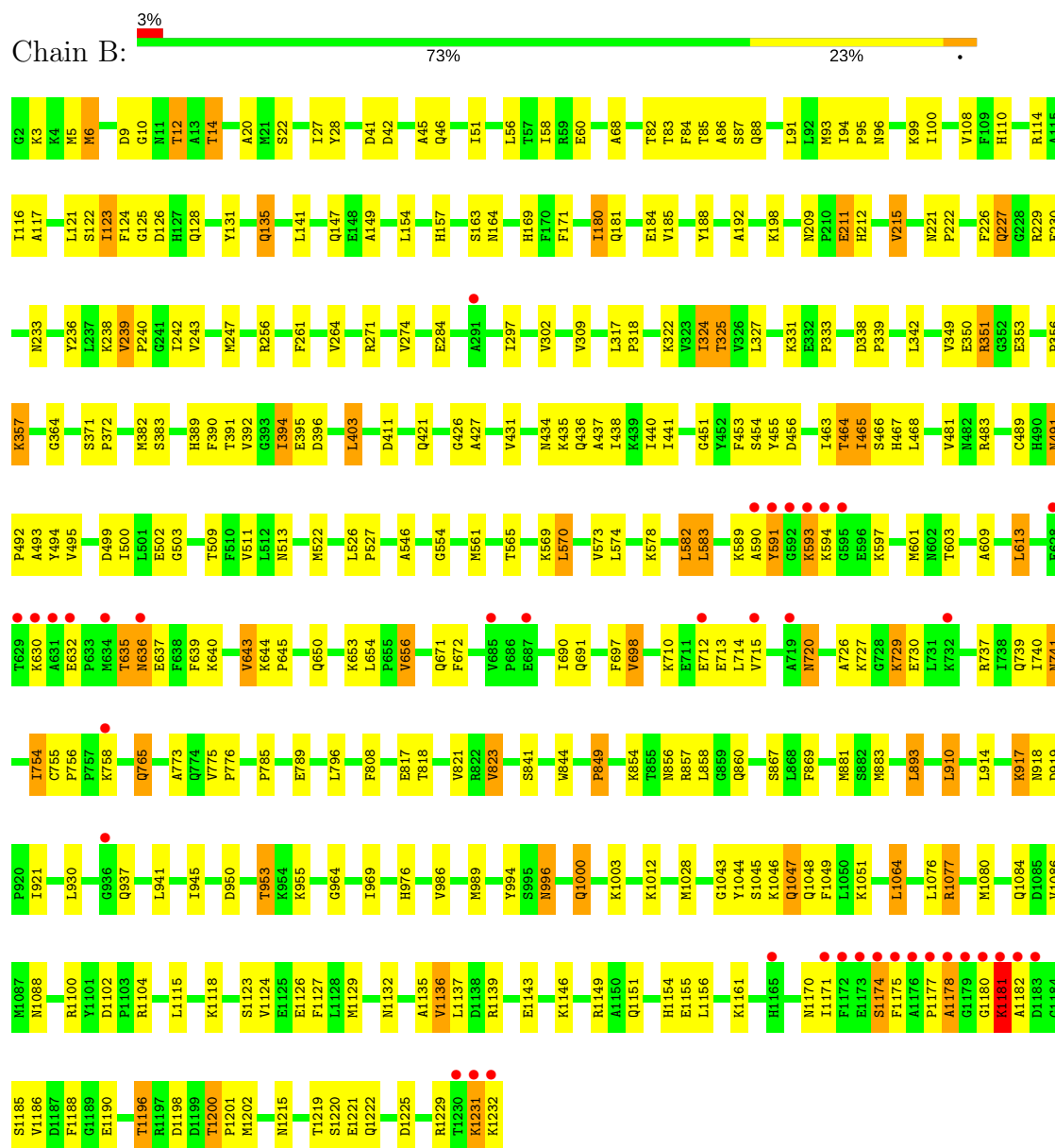
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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-FERREDOXIN OXIDOREDUCTASE



- Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.18Å 146.81Å 212.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 2.32 51.02 – 2.32	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.48-2.32) 96.3 (51.02-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.238 0.184 , 0.234	Depositor DCC
R_{free} test set	5682 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19646	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, PYR, CA, 2TP

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	0/9585	0.67	3/12954 (0.0%)
1	B	0.43	0/9585	0.68	2/12954 (0.0%)
All	All	0.42	0/19170	0.67	5/25908 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLY	N-CA-C	6.16	128.49	113.10
1	B	364	GLY	N-CA-C	6.14	128.44	113.10
1	A	125	GLY	N-CA-C	5.95	127.98	113.10
1	A	364	GLY	N-CA-C	5.23	126.17	113.10
1	A	141	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

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	9383	0	9262	324	0
1	B	9383	0	9262	329	0
2	A	24	0	0	1	0
2	B	24	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	16	1	0
3	B	27	0	15	2	0
4	A	6	0	3	1	0
4	B	6	0	3	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	327	0	0	5	0
7	B	435	0	0	10	0
All	All	19646	0	18561	610	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 16.

All (610) 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)
3:A:2236:2TP:O4'	3:A:2236:2TP:N4'	1.59	1.35
3:B:2236:2TP:O4'	3:B:2236:2TP:N4'	1.68	1.27
1:B:1132:ASN:HD21	1:B:1139:ARG:HH12	1.04	1.02
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.39	1.01
1:B:123:ILE:HD13	1:B:123:ILE:H	1.25	1.01
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.25	0.99
1:B:639:PHE:HA	1:B:643:VAL:HG13	1.46	0.96
1:A:1080:MET:H	1:B:1215:ASN:ND2	1.65	0.94
1:B:227:GLN:HE21	1:B:227:GLN:H	1.16	0.91
1:B:1181:LYS:HD2	1:B:1182:ALA:H	1.31	0.90
1:B:1124:VAL:HG11	1:B:1156:LEU:HD21	1.54	0.89
1:B:454:SER:HB3	1:B:465:ILE:HG23	1.55	0.88
1:A:398:VAL:HG13	1:A:656:VAL:HG22	1.58	0.84
1:A:1077:ARG:HH11	1:A:1077:ARG:HB2	1.43	0.83
1:A:157:HIS:O	1:A:161:ILE:HD13	1.79	0.82
1:B:396:ASP:HA	1:B:656:VAL:CG1	2.09	0.82
1:B:593:LYS:HD2	1:B:594:LYS:N	1.94	0.81
1:B:817:GLU:HB3	1:B:989:MET:CE	2.10	0.81
1:A:436:GLN:O	1:A:440:ILE:HG12	1.80	0.81
1:B:351:ARG:HD3	1:B:353:GLU:HB2	1.62	0.81
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.62	0.80
1:A:986:VAL:HG23	1:A:1064:LEU:HD23	1.63	0.80
1:B:817:GLU:HB3	1:B:989:MET:HE2	1.62	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:MET:H	1:B:1215:ASN:HD21	1.25	0.79
1:B:1219:THR:HB	1:B:1222:GLN:HG3	1.63	0.79
1:B:147:GLN:HE22	1:B:184:GLU:H	1.31	0.79
1:A:876:GLY:HA3	1:A:959:ILE:HD11	1.64	0.78
1:A:1230:THR:O	1:A:1232:LYS:HG2	1.82	0.78
1:A:639:PHE:HA	1:A:643:VAL:CG1	2.13	0.77
1:B:356:PRO:O	1:B:357:LYS:HB3	1.82	0.77
1:B:438:ILE:HD11	1:B:468:LEU:HD13	1.65	0.77
1:B:554:GLY:HA3	1:B:601:MET:HE2	1.67	0.76
1:A:10:GLY:O	1:A:14:THR:HG23	1.85	0.76
1:B:135:GLN:NE2	1:B:135:GLN:H	1.83	0.76
1:B:856:ASN:HD21	1:B:860:GLN:HE21	1.34	0.75
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.35	0.75
1:B:986:VAL:HG22	1:B:1064:LEU:HD23	1.68	0.75
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.35	0.74
1:B:635:THR:HG23	1:B:636:ASN:N	2.00	0.74
1:B:1077:ARG:HH11	1:B:1077:ARG:HB2	1.52	0.74
1:A:737:ARG:HH11	1:A:739:GLN:HE22	1.35	0.74
1:A:691:GLN:HE22	1:A:727:LYS:H	1.35	0.73
1:B:322:LYS:O	1:B:356:PRO:O	2.06	0.73
1:B:1181:LYS:CD	1:B:1182:ALA:H	2.01	0.73
1:A:196:ASN:OD1	1:A:198:LYS:HD2	1.88	0.73
1:A:128:GLN:HE22	1:B:229:ARG:HE	1.34	0.73
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.88	0.73
1:A:238:LYS:O	1:A:242:ILE:HD13	1.87	0.73
1:A:509:THR:HG22	1:A:540:LYS:HD2	1.69	0.73
1:A:876:GLY:HA3	1:A:959:ILE:CD1	2.19	0.73
1:B:463:ILE:HD12	1:B:464:THR:H	1.52	0.73
1:A:227:GLN:HE21	1:A:227:GLN:H	1.37	0.73
1:B:110:HIS:HD2	1:B:169:HIS:CD2	2.08	0.72
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.72	0.72
1:B:893:LEU:HB3	1:B:945:ILE:HD11	1.72	0.72
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.89	0.72
1:B:1132:ASN:O	1:B:1136:VAL:HG22	1.90	0.71
1:A:902:ALA:O	1:A:907:LYS:HE3	1.89	0.71
1:A:1123:SER:O	1:A:1126:GLU:HG2	1.90	0.71
1:B:494:TYR:HB3	1:B:500:ILE:HD11	1.72	0.71
1:A:1076:LEU:HD13	1:A:1086:VAL:HG21	1.73	0.71
1:A:1174:SER:H	1:B:1154:HIS:HE1	1.38	0.71
1:A:637:GLU:CD	1:A:637:GLU:H	1.94	0.70
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLN:HE22	1:A:184:GLU:H	1.36	0.70
1:B:1219:THR:HG22	1:B:1220:SER:N	2.06	0.70
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.74	0.70
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.74	0.70
1:A:434:ASN:O	1:A:438:ILE:HG12	1.91	0.69
1:B:9:ASP:OD2	1:B:12:THR:HG23	1.92	0.69
1:A:1132:ASN:HD21	1:A:1139:ARG:HH12	1.40	0.69
1:A:8:THR:HB	1:A:12:THR:OG1	1.92	0.69
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.10	0.68
1:B:227:GLN:NE2	1:B:227:GLN:H	1.91	0.68
1:A:1219:THR:HG21	7:B:2281:HOH:O	1.94	0.68
1:A:9:ASP:OD2	1:A:12:THR:HG23	1.94	0.68
1:A:455:TYR:HB2	1:B:1201:PRO:HG3	1.76	0.68
1:B:593:LYS:CD	1:B:594:LYS:HG3	2.23	0.68
1:B:391:THR:HB	1:B:394:ILE:HD11	1.76	0.67
1:B:123:ILE:CD1	1:B:123:ILE:H	2.03	0.67
1:A:264:VAL:HG21	1:A:284:GLU:OE1	1.93	0.67
1:A:1231:LYS:HG3	1:A:1232:LYS:N	2.06	0.67
1:B:1200:THR:CG2	1:B:1202:MET:H	2.07	0.67
1:B:180:ILE:HD11	1:B:438:ILE:HG21	1.76	0.67
1:A:279:SER:O	1:A:283:ILE:HG12	1.95	0.66
1:B:110:HIS:CD2	1:B:169:HIS:HD2	2.14	0.66
1:B:1132:ASN:ND2	1:B:1139:ARG:HH12	1.84	0.66
1:B:356:PRO:O	1:B:357:LYS:CB	2.42	0.65
1:A:691:GLN:NE2	1:A:727:LYS:H	1.95	0.65
1:B:436:GLN:O	1:B:440:ILE:HG12	1.97	0.65
1:A:1200:THR:CG2	1:A:1202:MET:H	2.10	0.64
1:B:396:ASP:HA	1:B:656:VAL:HG11	1.79	0.64
1:B:737:ARG:HH11	1:B:739:GLN:HE22	1.43	0.64
1:A:1180:GLY:O	1:A:1181:LYS:HB2	1.97	0.64
1:B:394:ILE:H	1:B:394:ILE:HD13	1.63	0.64
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.79	0.64
1:B:464:THR:HG23	7:B:2187:HOH:O	1.97	0.64
1:B:5:MET:CE	1:B:184:GLU:HB2	2.27	0.64
1:B:5:MET:HE1	1:B:184:GLU:HB2	1.79	0.64
1:B:463:ILE:HD13	1:B:494:TYR:CE1	2.34	0.63
1:B:464:THR:HG21	7:B:2171:HOH:O	1.98	0.63
1:B:6:MET:CE	1:B:185:VAL:HG11	2.28	0.63
1:B:1047:GLN:CD	1:B:1047:GLN:H	2.02	0.63
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.98	0.63
1:B:1200:THR:HG22	1:B:1202:MET:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:VAL:HB	1:B:776:PRO:HD3	1.81	0.62
1:A:921:ILE:H	1:A:921:ILE:HD12	1.64	0.62
1:B:917:LYS:HB3	1:B:917:LYS:HZ3	1.65	0.62
1:A:1077:ARG:NH1	1:A:1077:ARG:HB2	2.15	0.62
1:B:271:ARG:HD3	1:B:383:SER:HB3	1.82	0.62
1:B:910:LEU:HD13	1:B:930:LEU:HD11	1.81	0.62
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.99	0.62
1:A:1198:ASP:OD2	1:A:1200:THR:HB	1.99	0.61
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.29	0.61
1:B:10:GLY:O	1:B:14:THR:HG23	2.00	0.61
1:A:287:ILE:HD11	1:A:379:TYR:OH	2.01	0.61
1:B:609:ALA:O	1:B:613:LEU:HD22	2.01	0.60
1:A:594:LYS:HB2	1:A:598:ILE:HD12	1.83	0.60
1:A:396:ASP:HA	1:A:656:VAL:HG13	1.83	0.60
1:B:1231:LYS:O	1:B:1232:LYS:HB2	2.00	0.60
1:B:1151:GLN:O	1:B:1155:GLU:HG3	2.01	0.60
1:A:1080:MET:N	1:B:1215:ASN:HD21	1.98	0.60
1:B:1219:THR:CG2	1:B:1220:SER:N	2.64	0.60
1:B:691:GLN:HE22	1:B:726:ALA:HA	1.66	0.60
1:A:180:ILE:HD11	1:A:438:ILE:HG21	1.84	0.60
1:A:730:GLU:CD	1:A:730:GLU:H	2.04	0.60
1:B:1200:THR:HG22	1:B:1202:MET:N	2.17	0.59
1:B:14:THR:HG21	1:B:171:PHE:CE2	2.37	0.59
1:B:573:VAL:HG23	1:B:574:LEU:HG	1.83	0.59
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.83	0.59
1:B:392:VAL:HG22	1:B:403:LEU:HD22	1.84	0.59
1:A:128:GLN:NE2	1:B:229:ARG:HE	2.00	0.59
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.00	0.59
1:A:297:ILE:HB	1:A:379:TYR:CE2	2.37	0.59
1:B:1124:VAL:HG11	1:B:1156:LEU:CD2	2.30	0.59
1:A:394:ILE:HD13	1:A:394:ILE:H	1.66	0.59
1:A:283:ILE:O	1:A:287:ILE:HG12	2.03	0.59
1:A:99:LYS:HE3	1:B:867:SER:O	2.03	0.59
1:B:1129:MET:CE	1:B:1149:ARG:HD3	2.32	0.59
1:B:437:ALA:O	1:B:441:ILE:HG12	2.03	0.58
1:A:917:LYS:HG3	1:A:918:ASN:N	2.19	0.58
1:A:331:LYS:HE3	1:B:230:GLU:OE2	2.03	0.58
1:B:27:ILE:HG13	1:B:28:TYR:N	2.18	0.58
1:B:396:ASP:HA	1:B:656:VAL:HG12	1.86	0.58
1:A:357:LYS:HE3	1:A:359:LEU:HD11	1.84	0.58
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:N	1:B:123:ILE:HD13	2.07	0.58
1:B:463:ILE:HD12	1:B:464:THR:N	2.19	0.58
1:B:593:LYS:HD2	1:B:594:LYS:HG3	1.83	0.58
1:B:82:THR:HG23	1:B:108:VAL:O	2.04	0.58
1:B:1143:GLU:O	1:B:1146:LYS:HG2	2.04	0.58
1:B:893:LEU:HB3	1:B:945:ILE:CD1	2.33	0.58
1:A:709:ALA:HB3	1:A:714:LEU:HD11	1.84	0.57
1:A:467:HIS:CD2	1:A:481:VAL:H	2.23	0.57
1:A:986:VAL:CG2	1:A:1064:LEU:HA	2.34	0.57
1:A:1171:ILE:HD12	1:B:1161:LYS:HD3	1.86	0.57
7:A:2075:HOH:O	1:B:953:THR:HG21	2.04	0.57
1:A:227:GLN:NE2	1:A:227:GLN:H	2.03	0.57
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.86	0.57
1:B:135:GLN:HE21	1:B:135:GLN:H	1.51	0.57
1:A:1188:PHE:CE1	1:A:1196:THR:HG23	2.40	0.57
1:B:198:LYS:H	1:B:198:LYS:HD2	1.70	0.57
1:A:198:LYS:H	1:A:198:LYS:HD2	1.70	0.57
1:B:82:THR:HG22	1:B:83:THR:H	1.69	0.57
1:B:817:GLU:HB3	1:B:989:MET:HE3	1.85	0.57
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.86	0.57
1:B:467:HIS:CD2	1:B:481:VAL:H	2.23	0.56
1:A:1029:VAL:HG22	1:A:1037:VAL:HG21	1.87	0.56
1:B:630:LYS:O	1:B:630:LYS:HG3	2.06	0.56
1:A:110:HIS:CD2	1:A:169:HIS:HD2	2.19	0.56
1:A:794:ASP:OD1	1:A:1054:LYS:HD2	2.04	0.56
1:A:1166:MET:O	1:A:1169:THR:HG22	2.05	0.56
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.88	0.56
1:A:1215:ASN:ND2	1:B:1080:MET:H	2.03	0.56
1:A:1024:ASP:OD2	1:A:1027:ARG:HG3	2.05	0.56
1:A:82:THR:HG22	1:A:108:VAL:O	2.05	0.56
1:B:1177:PRO:O	1:B:1178:ALA:HB2	2.05	0.56
1:A:467:HIS:HD2	1:A:481:VAL:H	1.52	0.56
1:A:1080:MET:N	1:B:1215:ASN:ND2	2.47	0.56
1:B:463:ILE:HD13	1:B:494:TYR:CZ	2.41	0.56
1:A:910:LEU:HD13	1:A:930:LEU:HD11	1.86	0.56
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.86	0.56
1:A:501:LEU:O	1:A:504:ILE:HG22	2.05	0.56
1:B:325:THR:CG2	1:B:382:MET:SD	2.93	0.56
1:A:986:VAL:HG22	1:A:1064:LEU:HA	1.88	0.55
1:A:426:GLY:O	1:A:427:ALA:HB3	2.07	0.55
1:A:520:GLU:HG3	1:A:521:ASP:N	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1200:THR:CG2	1:B:1202:MET:HB2	2.37	0.55
1:A:222:PRO:HD3	1:B:124:PHE:CE2	2.42	0.55
1:A:710:LYS:O	1:A:712:GLU:N	2.39	0.55
1:B:1077:ARG:NH1	1:B:1077:ARG:HB2	2.19	0.55
1:B:42:ASP:O	1:B:46:GLN:HG3	2.06	0.55
1:A:1051:LYS:HE3	1:A:1100:ARG:NH1	2.22	0.55
1:A:1200:THR:HG22	1:A:1202:MET:H	1.72	0.55
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.42	0.55
1:A:918:ASN:HA	1:A:954:LYS:HD2	1.87	0.55
1:B:264:VAL:HG11	1:B:284:GLU:HG3	1.88	0.55
1:B:636:ASN:HD22	1:B:672:PHE:HE1	1.54	0.55
1:B:737:ARG:HE	1:B:739:GLN:NE2	2.04	0.55
1:A:1019:ARG:HH12	1:B:1181:LYS:H	1.54	0.55
1:A:325:THR:HG21	7:A:2145:HOH:O	2.06	0.55
1:A:331:LYS:HD3	1:A:362:ARG:CZ	2.37	0.55
1:A:534:ILE:HD13	1:A:539:LEU:HD12	1.89	0.55
1:B:741:ASN:C	1:B:741:ASN:HD22	2.09	0.55
1:A:1200:THR:HG23	1:A:1202:MET:HE2	1.88	0.55
1:A:1200:THR:CG2	1:A:1202:MET:HB2	2.37	0.55
1:B:110:HIS:HE1	1:B:157:HIS:NE2	2.05	0.55
1:B:438:ILE:CD1	1:B:468:LEU:HD13	2.34	0.55
1:A:530:ILE:O	1:A:534:ILE:HG12	2.07	0.54
1:A:921:ILE:N	1:A:921:ILE:HD12	2.21	0.54
1:A:554:GLY:HA3	1:A:601:MET:HE2	1.89	0.54
1:B:1129:MET:HE2	1:B:1149:ARG:HD3	1.88	0.54
1:A:841:SER:HA	1:A:844:TRP:CE2	2.42	0.54
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.43	0.54
1:B:1232:LYS:NZ	1:B:1232:LYS:HB3	2.22	0.54
1:B:227:GLN:HE21	1:B:227:GLN:N	1.94	0.54
1:B:499:ASP:OD2	1:B:502:GLU:HB2	2.08	0.54
1:A:391:THR:OG1	1:A:394:ILE:HD11	2.07	0.54
1:B:690:ILE:HG12	2:B:2233:SF4:S2	2.47	0.54
1:A:1188:PHE:HE1	1:A:1196:THR:HG23	1.73	0.54
1:A:283:ILE:HD13	1:A:375:VAL:HG22	1.89	0.54
1:B:243:VAL:O	1:B:247:MET:HG3	2.07	0.54
1:B:6:MET:HE2	1:B:185:VAL:HG11	1.89	0.54
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.42	0.54
1:A:273:ILE:HD11	1:A:378:VAL:CG1	2.38	0.54
1:A:714:LEU:N	1:A:714:LEU:HD12	2.23	0.54
1:B:394:ILE:N	1:B:394:ILE:HD13	2.22	0.54
1:A:712:GLU:O	1:A:715:VAL:HG23	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ILE:HD12	1:A:418:ILE:N	2.24	0.53
1:B:1219:THR:HG22	1:B:1221:GLU:H	1.73	0.53
1:A:906:VAL:HG12	1:A:910:LEU:HD22	1.90	0.53
1:B:591:TYR:C	1:B:593:LYS:H	2.10	0.53
1:A:322:LYS:O	1:A:356:PRO:O	2.27	0.53
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	1.90	0.53
1:B:1132:ASN:HD21	1:B:1139:ARG:NH1	1.89	0.53
1:A:325:THR:CG2	1:A:382:MET:SD	2.97	0.53
1:A:345:CYS:SG	1:B:349:VAL:HG21	2.49	0.53
1:A:350:GLU:CD	1:B:389:HIS:HE1	2.12	0.53
1:A:759:GLU:CD	1:A:759:GLU:H	2.11	0.53
1:B:917:LYS:NZ	1:B:917:LYS:CB	2.72	0.53
1:A:1077:ARG:CB	1:A:1077:ARG:HH11	2.19	0.53
1:A:1201:PRO:HG3	1:B:455:TYR:HB2	1.91	0.53
1:B:996:ASN:ND2	3:B:2236:2TP:S1	2.82	0.53
1:A:1200:THR:HG22	1:A:1202:MET:N	2.23	0.52
1:B:591:TYR:C	1:B:593:LYS:N	2.61	0.52
1:A:398:VAL:CG1	1:A:656:VAL:HG22	2.33	0.52
1:B:6:MET:HE3	1:B:185:VAL:HG11	1.92	0.52
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.92	0.52
1:B:238:LYS:O	1:B:242:ILE:HG12	2.08	0.52
1:B:697:PHE:CD2	1:B:1046:LYS:HD3	2.44	0.52
1:A:986:VAL:HG22	1:A:1063:SER:O	2.10	0.52
1:A:1124:VAL:HG22	7:A:2292:HOH:O	2.10	0.52
1:A:3:LYS:HD3	1:A:184:GLU:OE1	2.09	0.52
1:A:698:VAL:HG13	7:A:2291:HOH:O	2.09	0.52
1:B:147:GLN:NE2	1:B:184:GLU:H	2.04	0.52
1:B:391:THR:CB	1:B:394:ILE:HD11	2.40	0.52
1:B:635:THR:CG2	1:B:640:LYS:HG3	2.40	0.52
1:A:491:ASN:HD22	1:A:491:ASN:C	2.13	0.52
1:B:491:ASN:HD22	1:B:491:ASN:C	2.14	0.52
1:A:700:PRO:HG2	1:A:814:GLY:HA2	1.91	0.52
1:B:1044:TYR:OH	1:B:1118:LYS:HE2	2.09	0.52
1:B:754:ILE:HG12	7:B:2383:HOH:O	2.09	0.52
1:A:593:LYS:HG3	1:A:594:LYS:N	2.24	0.52
1:B:180:ILE:HD13	1:B:451:GLY:N	2.25	0.52
1:A:950:ASP:OD2	1:B:212:HIS:HE1	1.93	0.52
1:B:554:GLY:HA3	1:B:601:MET:CE	2.40	0.52
1:A:754:ILE:HD12	1:A:1084:GLN:CB	2.40	0.51
1:A:737:ARG:HE	1:A:739:GLN:HE21	1.57	0.51
1:B:561:MET:CE	1:B:583:LEU:HD21	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:ASN:HB3	1:B:639:PHE:H	1.75	0.51
1:B:729:LYS:C	1:B:729:LYS:HD3	2.31	0.51
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.09	0.51
1:A:501:LEU:HD22	1:A:530:ILE:HD12	1.91	0.51
1:A:566:ALA:HA	1:A:613:LEU:CD2	2.40	0.51
1:A:856:ASN:HD21	1:A:860:GLN:HE21	1.57	0.51
1:B:593:LYS:HD2	1:B:594:LYS:H	1.74	0.51
1:A:535:ALA:HB1	1:A:623:LYS:HG2	1.92	0.51
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.75	0.51
1:B:917:LYS:NZ	1:B:917:LYS:HB3	2.25	0.51
1:A:229:ARG:HE	1:B:128:GLN:HE22	1.57	0.51
1:B:569:LYS:HG2	1:B:570:LEU:HD12	1.92	0.51
1:A:1200:THR:HG23	1:A:1202:MET:CE	2.41	0.51
1:A:121:LEU:HD23	1:A:121:LEU:C	2.30	0.51
1:A:910:LEU:O	1:A:914:LEU:HD22	2.11	0.51
1:B:594:LYS:NZ	1:B:594:LYS:HB3	2.26	0.51
1:B:1188:PHE:HE1	1:B:1196:THR:HG23	1.75	0.51
1:A:1107:ALA:HB2	1:A:1175:PHE:HB3	1.93	0.51
1:B:27:ILE:CG1	1:B:28:TYR:N	2.73	0.51
1:A:2:GLY:N	1:A:187:ASP:OD2	2.44	0.51
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.93	0.50
1:A:524:LYS:HD2	1:A:525:HIS:CE1	2.45	0.50
1:B:773:ALA:O	1:B:776:PRO:HD2	2.10	0.50
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.41	0.50
1:B:27:ILE:HD12	1:B:28:TYR:H	1.76	0.50
1:A:5:MET:HE2	1:A:184:GLU:HG3	1.92	0.50
1:A:58:ILE:N	1:A:58:ILE:HD12	2.26	0.50
1:B:609:ALA:O	1:B:613:LEU:CD2	2.59	0.50
1:B:82:THR:HG22	1:B:83:THR:N	2.26	0.50
1:A:986:VAL:CG2	1:A:1064:LEU:HD23	2.36	0.50
1:A:754:ILE:HD12	1:A:1084:GLN:HB3	1.93	0.50
1:A:87:SER:HB2	1:A:114:ARG:HG2	1.93	0.50
1:B:325:THR:HG22	1:B:382:MET:SD	2.51	0.50
1:B:1200:THR:HG21	1:B:1202:MET:HB2	1.94	0.50
1:B:121:LEU:C	1:B:121:LEU:HD23	2.32	0.50
1:A:198:LYS:CD	1:A:198:LYS:H	2.24	0.50
1:B:1198:ASP:OD2	1:B:1200:THR:HB	2.12	0.50
1:B:796:LEU:HD23	1:B:796:LEU:C	2.32	0.50
1:A:438:ILE:HD11	1:A:468:LEU:HD22	1.94	0.49
1:B:737:ARG:HE	1:B:739:GLN:HE21	1.59	0.49
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HD13	1:B:84:PHE:H	1.77	0.49
1:A:273:ILE:HD11	1:A:378:VAL:HG12	1.93	0.49
1:B:467:HIS:HB3	1:B:481:VAL:HG23	1.94	0.49
1:B:643:VAL:HB	1:B:849:PRO:HB2	1.94	0.49
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.10	0.49
1:B:1171:ILE:N	1:B:1171:ILE:HD12	2.27	0.49
1:A:602:ASN:O	1:A:606:VAL:HG23	2.12	0.49
1:B:209:ASN:OD1	1:B:211:GLU:HB2	2.12	0.49
1:B:650:GLN:NE2	1:B:653:LYS:NZ	2.60	0.49
1:A:565:THR:HG21	1:A:609:ALA:HB3	1.93	0.49
1:B:1123:SER:O	1:B:1126:GLU:HG2	2.12	0.49
1:A:591:TYR:C	1:A:593:LYS:H	2.15	0.49
1:A:487:VAL:HG23	1:A:504:ILE:HD13	1.95	0.48
1:B:96:ASN:O	1:B:100:ILE:HG13	2.13	0.48
1:B:565:THR:HG21	1:B:609:ALA:HB3	1.95	0.48
1:B:720:ASN:H	1:B:720:ASN:ND2	2.11	0.48
1:A:444:ASN:HB2	1:A:582:LEU:HD21	1.95	0.48
1:A:94:ILE:HB	1:A:95:PRO:HD3	1.94	0.48
1:B:1077:ARG:HH11	1:B:1077:ARG:CB	2.25	0.48
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.29	0.48
1:B:491:ASN:ND2	1:B:493:ALA:H	2.11	0.48
1:B:88:GLN:HB3	7:B:2319:HOH:O	2.13	0.48
1:A:235:TYR:O	1:A:239:VAL:HG12	2.12	0.48
1:A:918:ASN:CA	1:A:954:LYS:HD2	2.44	0.48
1:B:964:GLY:HA2	1:B:994:TYR:HE1	1.79	0.48
1:B:27:ILE:CD1	1:B:28:TYR:H	2.27	0.48
1:A:230:GLU:OE2	1:B:331:LYS:HE2	2.14	0.48
1:A:421:GLN:HA	1:A:466:SER:O	2.14	0.48
1:B:1124:VAL:O	1:B:1127:PHE:HB3	2.13	0.48
1:B:1219:THR:CG2	1:B:1220:SER:H	2.26	0.48
1:A:128:GLN:NE2	1:B:229:ARG:HH21	2.11	0.48
1:B:3:LYS:HE3	1:B:184:GLU:OE1	2.13	0.48
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.95	0.48
1:B:570:LEU:CD1	1:B:570:LEU:N	2.77	0.47
1:A:1028:MET:HE2	1:B:1028:MET:HE2	1.95	0.47
1:B:1045:SER:OG	1:B:1047:GLN:NE2	2.47	0.47
1:B:274:VAL:HG23	1:B:324:ILE:HD13	1.95	0.47
1:B:349:VAL:HG23	1:B:350:GLU:N	2.28	0.47
1:B:494:TYR:CB	1:B:500:ILE:HD11	2.41	0.47
1:A:692:CYS:O	1:A:693:ASN:HB2	2.14	0.47
1:A:774:GLN:HA	1:A:777:ASN:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:THR:HG21	1:A:1202:MET:HB2	1.96	0.47
1:A:411:ASP:HB2	1:A:483:ARG:HD2	1.95	0.47
1:B:1043:GLY:HA2	1:B:1084:GLN:NE2	2.28	0.47
1:B:27:ILE:CG1	1:B:28:TYR:H	2.28	0.47
1:B:1043:GLY:HA2	1:B:1084:GLN:HE21	1.80	0.47
1:B:698:VAL:HG22	1:B:1084:GLN:CD	2.34	0.47
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.14	0.47
1:A:577:GLU:OE1	1:A:577:GLU:HA	2.14	0.47
1:A:741:ASN:C	1:A:741:ASN:HD22	2.18	0.47
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.50	0.47
1:A:45:ALA:HB1	1:B:1185:SER:HB3	1.97	0.47
1:A:691:GLN:HE22	1:A:726:ALA:HA	1.78	0.47
1:A:917:LYS:HB3	1:A:917:LYS:NZ	2.30	0.47
1:B:325:THR:HG21	7:B:2153:HOH:O	2.13	0.47
1:A:522:MET:SD	1:A:526:LEU:HD22	2.54	0.47
1:B:1180:GLY:O	1:B:1182:ALA:N	2.48	0.47
1:B:14:THR:HG22	1:B:149:ALA:HB1	1.95	0.47
1:A:561:MET:HE1	1:A:583:LEU:HD21	1.97	0.47
1:B:317:LEU:HD22	1:B:318:PRO:HD2	1.96	0.47
1:A:121:LEU:HD23	1:A:122:SER:N	2.30	0.46
1:A:1025:LEU:O	1:A:1029:VAL:HG13	2.15	0.46
1:B:483:ARG:HA	1:B:503:GLY:O	2.15	0.46
1:A:774:GLN:HA	1:A:774:GLN:NE2	2.30	0.46
1:A:8:THR:HB	1:A:12:THR:HG1	1.81	0.46
1:A:1010:VAL:CG2	1:A:1137:LEU:HG	2.45	0.46
1:A:45:ALA:CB	1:B:1185:SER:HB3	2.46	0.46
1:B:324:ILE:HG13	1:B:324:ILE:O	2.15	0.46
1:B:56:LEU:HG	1:B:58:ILE:HG12	1.96	0.46
1:A:1200:THR:HG23	1:A:1202:MET:H	1.78	0.46
1:A:673:GLU:O	1:A:674:LYS:C	2.54	0.46
1:B:395:GLU:O	1:B:656:VAL:HG12	2.15	0.46
1:B:491:ASN:HD22	1:B:492:PRO:N	2.13	0.46
1:B:371:SER:HB2	1:B:372:PRO:HD2	1.98	0.46
1:B:434:ASN:O	1:B:438:ILE:HG12	2.15	0.46
1:A:128:GLN:HE22	1:B:229:ARG:NE	2.08	0.46
1:B:754:ILE:HD13	1:B:1084:GLN:HB2	1.98	0.46
1:A:913:TRP:CE3	1:A:914:LEU:HD13	2.51	0.45
1:B:114:ARG:NE	1:B:123:ILE:HA	2.31	0.45
1:A:275:SER:O	1:A:302:VAL:HG13	2.15	0.45
1:A:325:THR:HG23	1:A:382:MET:SD	2.57	0.45
1:A:491:ASN:HD22	1:A:492:PRO:CD	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:LYS:HD3	1:B:594:LYS:HG3	1.98	0.45
1:B:758:LYS:HE3	1:B:758:LYS:HB2	1.77	0.45
1:B:390:PHE:CD1	1:B:403:LEU:HD22	2.51	0.45
1:B:431:VAL:HG12	1:B:435:LYS:HE3	1.98	0.45
1:A:180:ILE:HD12	1:A:181:GLN:N	2.31	0.45
1:A:495:VAL:HG13	1:A:496:GLY:N	2.32	0.45
1:A:544:ILE:HG23	1:A:544:ILE:O	2.16	0.45
1:A:549:ILE:CD1	1:A:608:GLN:HE21	2.29	0.45
1:B:10:GLY:O	1:B:14:THR:CG2	2.65	0.45
1:B:121:LEU:HD23	1:B:122:SER:N	2.31	0.45
1:A:1185:SER:HB3	1:B:45:ALA:HB3	1.98	0.45
1:A:759:GLU:O	1:A:759:GLU:HG2	2.16	0.45
1:A:1214:GLN:O	1:A:1214:GLN:HG2	2.17	0.45
1:A:779:GLU:O	1:A:783:ARG:HD3	2.17	0.45
1:A:949:SER:HA	1:A:952:TYR:CE2	2.51	0.45
1:B:554:GLY:O	1:B:601:MET:HE1	2.16	0.45
1:A:1029:VAL:HG22	1:A:1037:VAL:CG2	2.46	0.45
1:A:465:ILE:O	1:A:465:ILE:HG13	2.16	0.45
1:B:1129:MET:HE3	1:B:1149:ARG:NH1	2.31	0.45
1:B:236:TYR:O	1:B:239:VAL:HG13	2.17	0.45
1:B:740:ILE:HD12	1:B:740:ILE:N	2.31	0.45
1:B:841:SER:HA	1:B:844:TRP:CE2	2.52	0.45
1:A:99:LYS:HE2	1:B:117:ALA:HB1	1.98	0.45
1:B:710:LYS:HG3	1:B:713:GLU:OE2	2.17	0.45
1:A:1198:ASP:CG	1:A:1200:THR:HB	2.38	0.45
1:A:264:VAL:HG21	1:A:284:GLU:CD	2.38	0.45
1:A:398:VAL:HG22	7:B:2092:HOH:O	2.17	0.45
1:B:1200:THR:HG23	1:B:1202:MET:H	1.80	0.45
1:B:818:THR:HA	1:B:821:VAL:HG22	1.99	0.45
1:A:1003:LYS:HZ2	1:B:976:HIS:HD2	1.64	0.44
1:A:345:CYS:O	1:A:349:VAL:HG13	2.17	0.44
1:A:273:ILE:CD1	1:A:378:VAL:HG11	2.47	0.44
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.82	0.44
1:A:953:THR:HG21	7:B:2075:HOH:O	2.16	0.44
1:B:331:LYS:O	1:B:333:PRO:HD3	2.16	0.44
1:B:635:THR:HG23	1:B:636:ASN:H	1.75	0.44
1:A:1124:VAL:HG11	1:A:1156:LEU:HD21	1.98	0.44
1:A:591:TYR:C	1:A:593:LYS:N	2.70	0.44
1:B:1180:GLY:O	1:B:1181:LYS:HD2	2.16	0.44
1:B:1181:LYS:HD2	1:B:1182:ALA:N	2.14	0.44
1:A:1185:SER:HB3	1:B:45:ALA:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.87	0.44
1:A:637:GLU:N	1:A:637:GLU:CD	2.68	0.44
1:A:756:PRO:HB2	1:A:757:PRO:CD	2.48	0.44
1:B:1051:LYS:HE2	1:B:1100:ARG:NH1	2.33	0.44
1:B:522:MET:SD	1:B:526:LEU:HD13	2.56	0.44
1:B:883:MET:CE	1:B:955:LYS:HG3	2.47	0.44
1:A:326:VAL:CG1	1:A:340:LEU:HG	2.47	0.44
1:A:690:ILE:HG12	2:A:2233:SF4:S2	2.58	0.44
1:A:667:LEU:HD12	1:B:215:VAL:HG12	2.00	0.44
1:B:569:LYS:C	1:B:570:LEU:HD12	2.38	0.44
1:B:953:THR:HG22	7:B:2340:HOH:O	2.16	0.44
1:A:495:VAL:CG1	1:A:496:GLY:N	2.80	0.44
1:A:650:GLN:CD	1:A:653:LYS:HZ3	2.20	0.44
1:B:68:ALA:HB2	1:B:93:MET:HG2	1.99	0.44
1:A:124:PHE:CE2	1:B:222:PRO:HD3	2.52	0.44
1:A:630:LYS:O	1:A:632:GLU:HG3	2.17	0.44
1:B:1177:PRO:O	1:B:1178:ALA:CB	2.66	0.44
1:B:421:GLN:HA	1:B:466:SER:O	2.18	0.44
1:B:729:LYS:HD2	1:B:730:GLU:HG3	2.00	0.44
1:A:227:GLN:HE21	1:A:227:GLN:N	2.11	0.44
1:B:644:LYS:N	1:B:645:PRO:CD	2.80	0.44
1:A:1012:LYS:O	1:A:1013:PHE:HB2	2.18	0.44
1:A:1219:THR:HB	1:A:1222:GLN:CD	2.39	0.44
1:A:163:SER:O	1:A:164:ASN:HB2	2.18	0.44
1:A:143:SER:OG	1:A:171:PHE:HB3	2.18	0.44
1:A:181:GLN:HB3	1:A:181:GLN:HE21	1.57	0.44
1:A:729:LYS:C	1:A:729:LYS:HD3	2.38	0.44
1:A:331:LYS:NZ	1:B:233:ASN:HD21	2.16	0.44
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.48	0.43
1:A:394:ILE:N	1:A:394:ILE:HD13	2.30	0.43
1:A:869:PHE:CE2	1:A:969:ILE:HG21	2.53	0.43
1:B:513:ASN:ND2	1:B:546:ALA:H	2.16	0.43
1:A:87:SER:HB2	1:A:114:ARG:CG	2.46	0.43
1:A:338:ASP:HB3	1:A:339:PRO:CD	2.48	0.43
1:B:765:GLN:HA	1:B:765:GLN:HE21	1.82	0.43
1:A:1129:MET:HE2	1:A:1149:ARG:HD3	2.00	0.43
1:A:1019:ARG:NH1	1:B:1181:LYS:H	2.15	0.43
1:B:221:ASN:HB3	1:B:222:PRO:HD2	2.00	0.43
1:A:398:VAL:HG13	1:A:656:VAL:CG2	2.41	0.43
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.17	0.43
1:B:1188:PHE:CE1	1:B:1196:THR:HG23	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HG13	1:B:28:TYR:H	1.84	0.43
1:B:94:ILE:HB	1:B:95:PRO:HD3	2.00	0.43
1:A:390:PHE:HB2	1:A:403:LEU:HD13	2.01	0.43
1:A:422:PHE:O	1:A:465:ILE:HA	2.17	0.43
1:A:730:GLU:CD	1:A:730:GLU:N	2.71	0.43
1:B:123:ILE:HD11	1:B:124:PHE:CE2	2.53	0.43
1:B:85:THR:O	1:B:86:ALA:HB2	2.18	0.43
1:B:941:LEU:O	1:B:945:ILE:HG12	2.18	0.43
1:A:115:ALA:HB2	1:A:126:ASP:OD1	2.19	0.43
1:A:617:LYS:HD3	1:A:617:LYS:HA	1.90	0.43
1:B:91:LEU:HD11	1:B:116:ILE:HD12	2.01	0.43
1:B:869:PHE:CE2	1:B:969:ILE:HG21	2.53	0.43
1:B:917:LYS:HG3	1:B:918:ASN:N	2.33	0.43
1:A:390:PHE:HE1	1:A:392:VAL:CG2	2.31	0.43
1:B:56:LEU:HD23	1:B:58:ILE:CD1	2.49	0.43
1:B:590:ALA:O	1:B:591:TYR:C	2.54	0.43
1:A:1047:GLN:N	1:A:1047:GLN:OE1	2.52	0.43
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	2.01	0.43
1:A:996:ASN:HD21	4:A:2237:PYR:H32	1.83	0.43
1:A:609:ALA:O	1:A:613:LEU:HB2	2.18	0.43
1:B:110:HIS:CD2	1:B:169:HIS:CD2	2.95	0.43
1:A:1219:THR:HB	1:A:1222:GLN:OE1	2.19	0.42
1:A:37:GLY:HA3	7:A:2009:HOH:O	2.19	0.42
1:B:126:ASP:OD2	1:B:128:GLN:HG3	2.19	0.42
1:B:671:GLN:NE2	1:B:854:LYS:HD2	2.33	0.42
1:A:1229:ARG:HH12	1:B:765:GLN:HE22	1.67	0.42
1:A:561:MET:CE	1:A:583:LEU:HD21	2.49	0.42
1:B:317:LEU:HA	1:B:318:PRO:HD3	1.93	0.42
1:B:426:GLY:O	1:B:427:ALA:HB3	2.19	0.42
1:B:919:ASP:OD1	1:B:921:ILE:HB	2.19	0.42
1:A:491:ASN:HD22	1:A:492:PRO:N	2.17	0.42
1:A:636:ASN:O	1:A:640:LYS:HB2	2.19	0.42
1:A:9:ASP:HA	1:A:179:GLU:O	2.20	0.42
1:B:212:HIS:HD2	7:B:2069:HOH:O	2.01	0.42
1:B:755:CYS:HA	1:B:756:PRO:HD3	1.81	0.42
1:A:463:ILE:HG13	1:A:463:ILE:O	2.17	0.42
1:B:20:ALA:HB2	1:B:188:TYR:CE2	2.55	0.42
1:A:509:THR:CG2	1:A:540:LYS:HD2	2.46	0.42
1:B:644:LYS:HB3	1:B:645:PRO:HD3	2.01	0.42
1:B:6:MET:HE2	1:B:185:VAL:HG21	2.02	0.42
1:B:131:TYR:CE2	1:B:339:PRO:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:HIS:HD2	1:B:481:VAL:HB	1.84	0.42
1:A:114:ARG:NE	1:A:123:ILE:HA	2.34	0.42
1:A:1181:LYS:O	1:A:1182:ALA:HB3	2.19	0.42
1:A:1008:GLY:HA2	1:A:1148:LEU:HD13	2.02	0.42
1:A:516:TRP:HB2	1:A:522:MET:HE1	2.02	0.42
1:A:26:ALA:HB3	1:A:71:VAL:HG23	2.00	0.42
1:B:823:VAL:CG2	1:B:1049:PHE:HE2	2.32	0.42
1:A:59:ARG:HB2	1:B:881:MET:HE3	2.02	0.42
1:A:222:PRO:HD3	1:B:124:PHE:CD2	2.54	0.42
1:A:233:ASN:HB2	1:A:234:PRO:HD3	2.01	0.42
1:A:554:GLY:HA3	1:A:601:MET:CE	2.49	0.42
1:A:867:SER:O	1:B:99:LYS:HE3	2.19	0.42
1:B:456:ASP:OD1	1:B:463:ILE:HG22	2.19	0.42
1:B:589:LYS:C	1:B:590:ALA:O	2.57	0.42
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.55	0.42
1:A:643:VAL:HB	1:A:849:PRO:HB2	2.01	0.42
1:B:857:ARG:HG3	1:B:858:LEU:CD1	2.50	0.42
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.50	0.41
1:A:729:LYS:HD3	1:A:730:GLU:N	2.34	0.41
1:B:1170:ASN:OD1	1:B:1171:ILE:HD12	2.20	0.41
1:B:184:GLU:CD	1:B:256:ARG:HH12	2.24	0.41
1:B:463:ILE:CD1	1:B:494:TYR:CE1	3.02	0.41
1:B:856:ASN:HD21	1:B:860:GLN:NE2	2.10	0.41
1:B:857:ARG:HG3	1:B:858:LEU:HD13	2.02	0.41
1:A:154:LEU:HD13	1:A:250:VAL:HG22	2.01	0.41
1:A:645:PRO:O	1:A:650:GLN:HB2	2.20	0.41
1:B:261:PHE:CE1	1:B:302:VAL:HB	2.55	0.41
1:A:129:ASP:OD2	1:A:130:ILE:N	2.53	0.41
1:A:243:VAL:O	1:A:247:MET:HG3	2.20	0.41
1:A:124:PHE:HE2	1:B:221:ASN:HD22	1.68	0.41
1:B:27:ILE:HD11	1:B:84:PHE:O	2.20	0.41
1:B:390:PHE:CE1	1:B:392:VAL:CG2	3.04	0.41
1:B:411:ASP:HB2	1:B:483:ARG:HD2	2.03	0.41
1:A:978:LEU:O	1:A:1062:PRO:HG2	2.20	0.41
1:A:357:LYS:HE3	1:A:359:LEU:CD1	2.49	0.41
1:A:538:LYS:HD2	1:A:538:LYS:N	2.36	0.41
1:A:61:MET:HG3	1:A:67:ALA:HA	2.01	0.41
1:A:883:MET:HE3	1:A:887:ARG:HD2	2.03	0.41
1:B:163:SER:O	1:B:164:ASN:HB2	2.19	0.41
1:B:489:CYS:SG	1:B:500:ILE:HD13	2.60	0.41
1:B:635:THR:HG22	1:B:640:LYS:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG21	1:A:239:VAL:HG11	2.03	0.41
1:A:390:PHE:CD1	1:A:403:LEU:HD22	2.56	0.41
1:A:554:GLY:C	1:A:556:GLY:H	2.23	0.41
1:B:1000:GLN:HA	1:B:1012:LYS:HB2	2.03	0.41
1:B:22:SER:OG	1:B:82:THR:OG1	2.25	0.41
1:A:1010:VAL:HG22	1:A:1137:LEU:HG	2.01	0.41
1:B:1219:THR:HG21	1:B:1221:GLU:CD	2.41	0.41
1:A:164:ASN:ND2	1:A:206:LYS:NZ	2.69	0.41
1:A:622:TRP:O	1:A:624:ASP:N	2.53	0.41
1:A:765:GLN:HE21	1:A:765:GLN:HA	1.85	0.41
1:B:198:LYS:HD2	1:B:198:LYS:N	2.35	0.41
1:B:495:VAL:CG1	1:B:527:PRO:HD3	2.51	0.41
1:B:597:LYS:O	1:B:601:MET:HG3	2.20	0.41
1:B:87:SER:OG	1:B:88:GLN:N	2.51	0.41
1:A:1047:GLN:CD	1:A:1047:GLN:H	2.24	0.41
1:A:198:LYS:H	1:A:198:LYS:HZ2	1.69	0.41
1:A:297:ILE:HD13	1:A:297:ILE:H	1.85	0.41
1:A:491:ASN:HD22	1:A:492:PRO:HD2	1.86	0.41
1:A:720:ASN:C	1:A:720:ASN:HD22	2.24	0.41
1:A:287:ILE:HD12	1:A:297:ILE:HG12	2.03	0.41
1:A:350:GLU:OE2	1:B:389:HIS:HE1	2.03	0.41
1:B:1047:GLN:NE2	1:B:1047:GLN:H	2.18	0.41
1:B:1132:ASN:HA	1:B:1135:ALA:HB3	2.03	0.41
1:B:1129:MET:HE2	1:B:1149:ARG:CD	2.51	0.41
1:B:271:ARG:HB2	1:B:297:ILE:HG22	2.03	0.41
1:B:431:VAL:HG13	1:B:453:PHE:CD2	2.56	0.41
1:B:775:VAL:CB	1:B:776:PRO:HD3	2.51	0.41
1:A:486:TYR:OH	1:A:511:VAL:HG11	2.22	0.40
1:A:56:LEU:O	1:A:58:ILE:HD12	2.21	0.40
1:A:522:MET:HG2	1:A:616:PHE:CZ	2.55	0.40
1:B:1186:VAL:HG23	1:B:1190:GLU:OE1	2.22	0.40
1:A:221:ASN:HD22	1:B:124:PHE:HE2	1.68	0.40
1:B:713:GLU:OE1	1:B:785:PRO:HD2	2.21	0.40
1:A:27:ILE:HG23	1:A:28:TYR:N	2.36	0.40
1:A:444:ASN:CB	1:A:582:LEU:HD21	2.51	0.40
1:A:396:ASP:HA	1:A:656:VAL:CG1	2.47	0.40
1:A:578:LYS:O	1:A:582:LEU:HB2	2.22	0.40
1:B:1174:SER:O	1:B:1175:PHE:HB2	2.21	0.40
1:B:51:ILE:HB	1:B:192:ALA:HB2	2.03	0.40
1:B:578:LYS:HG2	1:B:582:LEU:HD22	2.02	0.40
1:A:644:LYS:HB3	1:A:645:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:ASP:OD1	1:A:896:LYS:NZ	2.51	0.40
1:B:338:ASP:HB3	1:B:339:PRO:CD	2.51	0.40
1:B:712:GLU:O	1:B:715:VAL:HG23	2.21	0.40
1:B:821:VAL:HG21	1:B:844:TRP:CH2	2.57	0.40
1:A:1200:THR:HA	1:A:1201:PRO:HD3	1.93	0.40
1:A:1219:THR:HG23	1:A:1220:SER:N	2.37	0.40
1:A:283:ILE:HD11	1:A:370:PHE:CE1	2.56	0.40
1:A:283:ILE:HD13	1:A:375:VAL:CG2	2.52	0.40
1:A:632:GLU:O	1:A:632:GLU:CD	2.59	0.40
1:A:898:LEU:HD23	1:A:898:LEU:HA	1.96	0.40
1:A:976:HIS:HE1	1:B:60:GLU:O	2.05	0.40
1:B:240:PRO:HB3	1:B:309:VAL:HG21	2.03	0.40
1:B:691:GLN:HE22	1:B:727:LYS:H	1.69	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	1229/1231 (100%)	1161 (94%)	58 (5%)	10 (1%)	22	26
1	B	1229/1231 (100%)	1173 (95%)	50 (4%)	6 (0%)	32	39
All	All	2458/2462 (100%)	2334 (95%)	108 (4%)	16 (1%)	25	29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	GLU
1	A	1231	LYS
1	B	1178	ALA
1	B	1181	LYS
1	B	1231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1178	ALA
1	A	1181	LYS
1	B	1174	SER
1	A	357	LYS
1	A	579	ALA
1	B	357	LYS
1	A	4	LYS
1	A	760	LYS
1	A	87	SER
1	A	623	LYS
1	B	591	TYR

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	978/978 (100%)	911 (93%)	67 (7%)	18	23
1	B	978/978 (100%)	909 (93%)	69 (7%)	17	22
All	All	1956/1956 (100%)	1820 (93%)	136 (7%)	18	22

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	THR
1	A	141	LEU
1	A	154	LEU
1	A	180	ILE
1	A	181	GLN
1	A	194	LEU
1	A	198	LYS
1	A	215	VAL
1	A	226	PHE
1	A	227	GLN
1	A	264	VAL
1	A	290	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	ILE
1	A	302	VAL
1	A	317	LEU
1	A	324	ILE
1	A	325	THR
1	A	327	LEU
1	A	342	LEU
1	A	349	VAL
1	A	351	ARG
1	A	359	LEU
1	A	394	ILE
1	A	403	LEU
1	A	465	ILE
1	A	491	ASN
1	A	501	LEU
1	A	511	VAL
1	A	570	LEU
1	A	583	LEU
1	A	624	ASP
1	A	632	GLU
1	A	634	MET
1	A	643	VAL
1	A	654	LEU
1	A	710	LYS
1	A	720	ASN
1	A	729	LYS
1	A	741	ASN
1	A	778	LEU
1	A	789	GLU
1	A	805	LEU
1	A	808	PHE
1	A	823	VAL
1	A	849	PRO
1	A	858	LEU
1	A	893	LEU
1	A	910	LEU
1	A	914	LEU
1	A	917	LYS
1	A	942	LEU
1	A	953	THR
1	A	993	VAL
1	A	1000	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1047	GLN
1	A	1048	GLN
1	A	1064	LEU
1	A	1077	ARG
1	A	1088	ASN
1	A	1115	LEU
1	A	1124	VAL
1	A	1137	LEU
1	A	1183	ASP
1	A	1196	THR
1	A	1200	THR
1	A	1219	THR
1	A	1225	ASP
1	B	6	MET
1	B	12	THR
1	B	14	THR
1	B	123	ILE
1	B	135	GLN
1	B	141	LEU
1	B	154	LEU
1	B	180	ILE
1	B	181	GLN
1	B	211	GLU
1	B	215	VAL
1	B	226	PHE
1	B	227	GLN
1	B	239	VAL
1	B	324	ILE
1	B	325	THR
1	B	327	LEU
1	B	342	LEU
1	B	351	ARG
1	B	394	ILE
1	B	403	LEU
1	B	464	THR
1	B	465	ILE
1	B	491	ASN
1	B	509	THR
1	B	511	VAL
1	B	570	LEU
1	B	582	LEU
1	B	583	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	593	LYS
1	B	603	THR
1	B	613	LEU
1	B	632	GLU
1	B	635	THR
1	B	636	ASN
1	B	637	GLU
1	B	643	VAL
1	B	654	LEU
1	B	656	VAL
1	B	698	VAL
1	B	714	LEU
1	B	720	ASN
1	B	729	LYS
1	B	741	ASN
1	B	754	ILE
1	B	765	GLN
1	B	789	GLU
1	B	808	PHE
1	B	823	VAL
1	B	849	PRO
1	B	893	LEU
1	B	910	LEU
1	B	914	LEU
1	B	917	LYS
1	B	937	GLN
1	B	953	THR
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1064	LEU
1	B	1077	ARG
1	B	1088	ASN
1	B	1115	LEU
1	B	1136	VAL
1	B	1137	LEU
1	B	1181	LYS
1	B	1196	THR
1	B	1200	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	16	HIS
1	A	46	GLN
1	A	110	HIS
1	A	128	GLN
1	A	147	GLN
1	A	164	ASN
1	A	169	HIS
1	A	181	GLN
1	A	212	HIS
1	A	220	GLN
1	A	221	ASN
1	A	227	GLN
1	A	233	ASN
1	A	288	ASN
1	A	389	HIS
1	A	421	GLN
1	A	434	ASN
1	A	467	HIS
1	A	491	ASN
1	A	513	ASN
1	A	602	ASN
1	A	608	GLN
1	A	650	GLN
1	A	691	GLN
1	A	693	ASN
1	A	720	ASN
1	A	739	GLN
1	A	741	ASN
1	A	750	ASN
1	A	765	GLN
1	A	774	GLN
1	A	777	ASN
1	A	836	ASN
1	A	860	GLN
1	A	866	ASN
1	A	880	ASN
1	A	918	ASN
1	A	976	HIS
1	A	996	ASN
1	A	1000	GLN
1	A	1048	GLN
1	A	1084	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1088	ASN
1	A	1132	ASN
1	A	1154	HIS
1	A	1165	HIS
1	A	1215	ASN
1	B	11	ASN
1	B	16	HIS
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS
1	B	128	GLN
1	B	135	GLN
1	B	147	GLN
1	B	164	ASN
1	B	169	HIS
1	B	181	GLN
1	B	212	HIS
1	B	220	GLN
1	B	221	ASN
1	B	227	GLN
1	B	233	ASN
1	B	288	ASN
1	B	389	HIS
1	B	421	GLN
1	B	434	ASN
1	B	467	HIS
1	B	491	ASN
1	B	513	ASN
1	B	536	ASN
1	B	602	ASN
1	B	636	ASN
1	B	650	GLN
1	B	683	GLN
1	B	688	ASN
1	B	691	GLN
1	B	693	ASN
1	B	720	ASN
1	B	739	GLN
1	B	741	ASN
1	B	750	ASN
1	B	765	GLN
1	B	774	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	777	ASN
1	B	836	ASN
1	B	860	GLN
1	B	866	ASN
1	B	880	ASN
1	B	918	ASN
1	B	937	GLN
1	B	976	HIS
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1048	GLN
1	B	1084	GLN
1	B	1088	ASN
1	B	1108	GLN
1	B	1132	ASN
1	B	1154	HIS
1	B	1215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	SF4	A	2233	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	2234	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	2235	1	0,12,12	0.00	-	0,24,24	0.00	-
3	2TP	A	2236	5	22,28,28	4.62	12 (54%)	24,41,41	1.76	9 (37%)
4	PYR	A	2237	-	2,5,5	0.90	0	2,6,6	1.51	0
2	SF4	B	2233	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	2234	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	2235	1	0,12,12	0.00	-	0,24,24	0.00	-
3	2TP	B	2236	5	22,28,28	27.30	11 (50%)	24,41,41	2.97	10 (41%)
4	PYR	B	2237	-	2,5,5	1.15	0	2,6,6	1.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	2233	1	-	0/0/48/48	0/6/5/5
2	SF4	A	2234	1	-	0/0/48/48	0/6/5/5
2	SF4	A	2235	1	-	0/0/48/48	0/6/5/5
3	2TP	A	2236	5	-	0/16/19/19	0/2/2/2
4	PYR	A	2237	-	-	0/0/4/4	0/0/0/0
2	SF4	B	2233	1	-	0/0/48/48	0/6/5/5
2	SF4	B	2234	1	-	0/0/48/48	0/6/5/5
2	SF4	B	2235	1	-	0/0/48/48	0/6/5/5
3	2TP	B	2236	5	-	0/16/19/19	0/2/2/2
4	PYR	B	2237	-	-	0/0/4/4	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2236	2TP	C35-C5'	-6.11	1.38	1.51
3	A	2236	2TP	C4A-C4	2.06	1.54	1.49
3	A	2236	2TP	C2'-N1'	2.12	1.38	1.34
3	A	2236	2TP	C4'-N3'	2.49	1.38	1.34
3	B	2236	2TP	P1-O13	2.77	1.61	1.50
3	B	2236	2TP	C2'-N1'	2.91	1.39	1.34
3	B	2236	2TP	C6'-N1'	3.13	1.41	1.34
3	A	2236	2TP	C2A-C2'	3.21	1.59	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2236	2TP	C4'-N4'	3.61	1.43	1.36
3	A	2236	2TP	C2'-N3'	3.77	1.40	1.34
3	A	2236	2TP	C6'-N1'	4.07	1.43	1.34
3	A	2236	2TP	C6'-C5'	5.66	1.49	1.37
3	B	2236	2TP	C2'-N3'	5.72	1.44	1.34
3	B	2236	2TP	P2-O11	6.07	1.69	1.60
3	B	2236	2TP	C4'-N3'	6.39	1.45	1.34
3	A	2236	2TP	P2-O11	7.27	1.71	1.60
3	A	2236	2TP	C5'-C4'	7.34	1.48	1.41
3	A	2236	2TP	O4'-N4'	7.58	1.59	1.39
3	B	2236	2TP	C6'-C5'	7.95	1.54	1.37
3	B	2236	2TP	C4-N3	9.95	1.48	1.39
3	B	2236	2TP	O4'-N4'	11.14	1.68	1.39
3	A	2236	2TP	C4-N3	13.86	1.51	1.39
3	B	2236	2TP	C4'-N4'	126.14	3.81	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2236	2TP	N4'-C4'-N3'	-9.01	96.52	118.43
3	A	2236	2TP	N1'-C2'-N3'	-3.72	119.16	125.59
3	B	2236	2TP	N1'-C2'-N3'	-3.43	119.66	125.59
3	A	2236	2TP	C6'-C5'-C4'	-2.23	112.68	115.62
3	B	2236	2TP	C35-C5'-C6'	2.01	124.55	120.70
3	B	2236	2TP	C2A-C2'-N3'	2.11	120.65	117.20
3	A	2236	2TP	C2A-C2'-N1'	2.30	119.66	117.06
3	B	2236	2TP	C2A-C2'-N1'	2.32	119.68	117.06
3	A	2236	2TP	C2A-C2'-N3'	2.41	121.15	117.20
3	A	2236	2TP	C5A-C5-C4	2.50	129.44	127.43
3	A	2236	2TP	O4'-N4'-C4'	2.54	126.05	119.54
3	B	2236	2TP	C6'-N1'-C2'	2.57	120.33	115.88
3	A	2236	2TP	C4A-C4-N3	2.57	125.81	122.53
3	A	2236	2TP	C5'-C35-N3	2.59	117.66	113.33
3	B	2236	2TP	C4A-C4-N3	2.61	125.86	122.53
3	B	2236	2TP	C5'-C35-N3	2.75	117.93	113.33
3	A	2236	2TP	C6'-N1'-C2'	2.88	120.85	115.88
3	B	2236	2TP	C5A-C5-C4	4.02	130.66	127.43
3	B	2236	2TP	O4'-N4'-C4'	7.76	139.44	119.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2233	SF4	1	0
3	A	2236	2TP	1	0
4	A	2237	PYR	1	0
2	B	2233	SF4	1	0
3	B	2236	2TP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1231/1231 (100%)	0.15	82 (6%) 19 25	5, 21, 65, 98	0
1	B	1231/1231 (100%)	-0.13	39 (3%) 48 55	4, 15, 46, 94	0
All	All	2462/2462 (100%)	0.01	121 (4%) 30 38	4, 18, 59, 98	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	ALA	14.5
1	B	1178	ALA	10.1
1	A	1177	PRO	10.0
1	B	1232	LYS	8.4
1	B	1176	ALA	8.1
1	A	633	PRO	7.7
1	B	631	ALA	7.4
1	A	1178	ALA	6.9
1	B	1182	ALA	6.5
1	A	631	ALA	6.5
1	A	1175	PHE	6.4
1	A	594	LYS	6.0
1	B	1175	PHE	5.5
1	B	1177	PRO	5.4
1	A	595	GLY	5.3
1	A	1232	LYS	5.2
1	A	629	THR	5.2
1	A	626	PRO	5.0
1	A	627	ALA	4.9
1	A	1180	GLY	4.9
1	A	1179	GLY	4.8
1	B	1180	GLY	4.8
1	A	588	HIS	4.7
1	B	1179	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	576	PHE	4.6
1	A	634	MET	4.6
1	B	594	LYS	4.5
1	A	593	LYS	4.5
1	B	1231	LYS	4.2
1	A	596	GLU	4.2
1	A	619	PRO	4.1
1	A	628	GLU	4.0
1	A	630	LYS	4.0
1	B	1183	ASP	4.0
1	A	758	LYS	4.0
1	B	1181	LYS	3.9
1	B	1174	SER	3.8
1	B	590	ALA	3.8
1	B	593	LYS	3.6
1	A	611	THR	3.6
1	A	1182	ALA	3.6
1	A	1174	SER	3.6
1	B	628	GLU	3.5
1	A	591	TYR	3.5
1	A	598	ILE	3.5
1	A	632	GLU	3.5
1	A	1165	HIS	3.5
1	A	636	ASN	3.4
1	A	717	ALA	3.3
1	B	1173	GLU	3.2
1	A	592	GLY	3.2
1	A	590	ALA	3.1
1	A	535	ALA	3.1
1	A	621	SER	3.1
1	A	577	GLU	3.1
1	A	618	TYR	3.0
1	A	520	GLU	3.0
1	A	719	ALA	3.0
1	A	781	ALA	3.0
1	A	759	GLU	2.9
1	A	1170	ASN	2.9
1	A	1231	LYS	2.9
1	A	597	LYS	2.9
1	A	554	GLY	2.8
1	A	635	THR	2.8
1	A	1230	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	601	MET	2.8
1	B	715	VAL	2.8
1	B	634	MET	2.7
1	B	1230	THR	2.7
1	A	589	LYS	2.7
1	B	687	GLU	2.7
1	A	581	ASP	2.7
1	B	1171	ILE	2.7
1	B	632	GLU	2.6
1	A	2	GLY	2.6
1	B	1165	HIS	2.6
1	A	714	LEU	2.6
1	B	595	GLY	2.6
1	A	578	LYS	2.6
1	B	630	LYS	2.6
1	B	732	LYS	2.6
1	A	715	VAL	2.5
1	A	620	ASP	2.5
1	A	617	LYS	2.5
1	A	732	LYS	2.5
1	B	591	TYR	2.5
1	A	1228	LYS	2.5
1	A	729	LYS	2.4
1	A	1173	GLU	2.4
1	A	780	TYR	2.4
1	A	712	GLU	2.4
1	B	592	GLY	2.4
1	A	538	LYS	2.4
1	B	629	THR	2.4
1	A	532	ARG	2.3
1	A	727	LYS	2.3
1	B	936	GLY	2.3
1	A	582	LEU	2.3
1	A	1227	SER	2.3
1	A	720	ASN	2.3
1	A	600	LYS	2.3
1	B	1172	PHE	2.2
1	A	711	GLU	2.2
1	A	1169	THR	2.2
1	A	710	LYS	2.2
1	B	685	VAL	2.2
1	A	518	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	712	GLU	2.2
1	A	1118	LYS	2.2
1	A	552	ASP	2.1
1	B	636	ASN	2.1
1	A	553	VAL	2.1
1	A	707	VAL	2.1
1	A	623	LYS	2.1
1	B	291	ALA	2.0
1	B	719	ALA	2.0
1	B	758	LYS	2.0
1	A	935	ALA	2.0
1	A	505	LYS	2.0
1	A	624	ASP	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
4	PYR	A	2237	6/6	0.95	0.20	0.84	22,29,33,34	0
4	PYR	B	2237	6/6	0.96	0.19	0.71	17,19,21,22	0
3	2TP	A	2236	27/27	0.97	0.16	-0.08	12,17,24,38	0
3	2TP	B	2236	27/27	0.98	0.14	-0.53	6,12,21,31	0
6	CA	A	2239	1/1	0.99	0.08	-1.28	34,34,34,34	0
5	MG	B	2238	1/1	0.99	0.08	-1.80	1,1,1,1	0
2	SF4	B	2235	8/8	0.98	0.06	-1.98	9,13,14,14	0
5	MG	A	2238	1/1	0.99	0.09	-2.10	7,7,7,7	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SF4	B	2233	8/8	0.97	0.06	-2.15	18,20,23,23	0
6	CA	B	2239	1/1	0.98	0.08	-2.16	30,30,30,30	0
2	SF4	A	2233	8/8	0.95	0.08	-2.26	34,35,37,38	0
2	SF4	A	2234	8/8	0.96	0.06	-2.51	26,27,28,30	0
2	SF4	A	2235	8/8	0.97	0.05	-2.88	18,22,24,24	0
2	SF4	B	2234	8/8	0.98	0.05	-3.68	13,14,16,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.