Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:30 am BST

PDB ID	:	1WYT
Title	:	Crystal structure of glycine decarboxylase (P-protein) of the glycine cleavage system, in apo form
Authors	:	Nakai, T.; Nakagawa, N.; Maoka, N.; Masui, R.; Kuramitsu, S.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-02-17
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

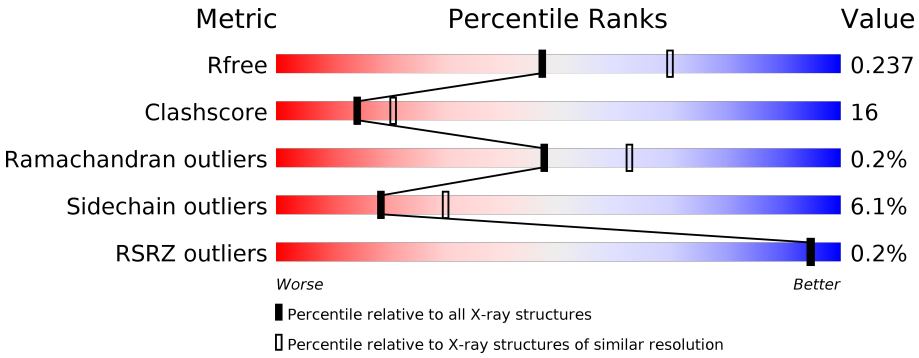
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	73% 24% .
1	C	438	73% 23% .
2	B	474	66% 30% . .
2	D	474	69% 28% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15062 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 glycine dehydrogenase (decarboxylating) subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			
1	C	437	Total	C	N	O	S	0	0	0
			3320	2129	575	607	9			

- Molecule 2 is a protein called glycine dehydrogenase subunit 2 (P-protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	471	Total	C	N	O	S	0	0	0
			3699	2373	653	661	12			
2	D	471	Total	C	N	O	S	0	0	0
			3699	2373	653	661	12			

- Molecule 3 is water.

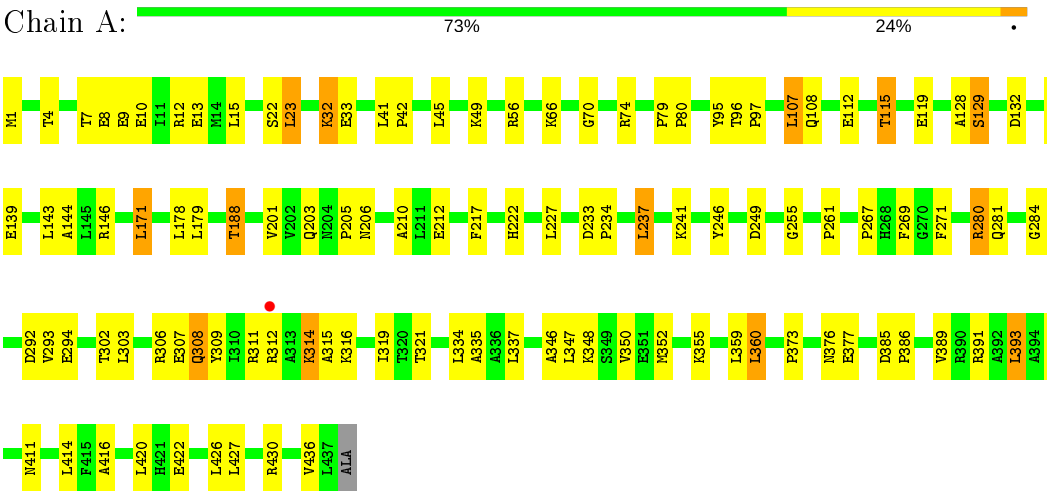
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	239	Total	O	0	0
			239	239		
3	B	312	Total	O	0	0
			312	312		
3	C	224	Total	O	0	0
			224	224		
3	D	249	Total	O	0	0
			249	249		

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 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.

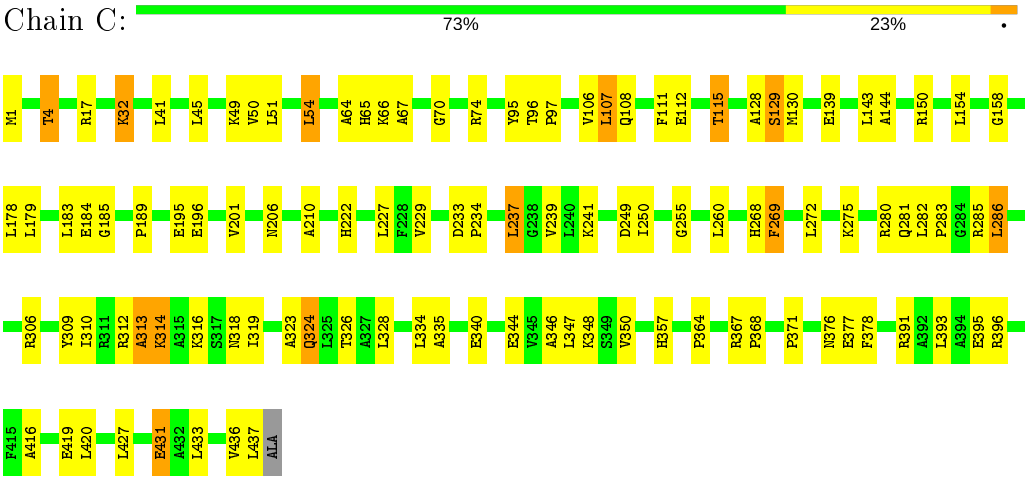
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

Chain A:



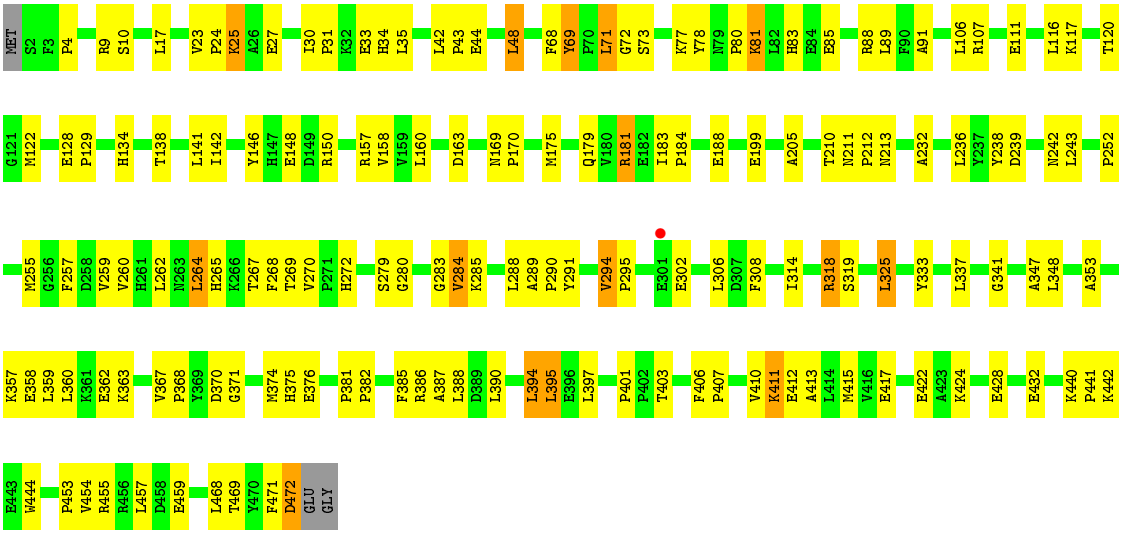
- Molecule 1: glycine dehydrogenase (decarboxylating) subunit 1

Chain C:



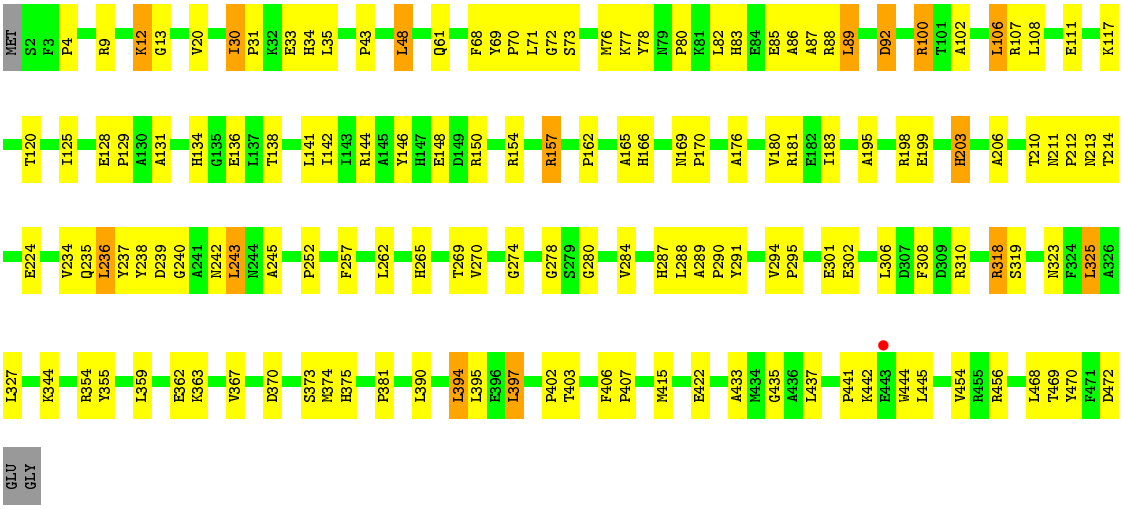
- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

Chain B:



- Molecule 2: glycine dehydrogenase subunit 2 (P-protein)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.55Å 89.55Å 371.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.35 – 2.40 48.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.35-2.40) 99.9 (48.35-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.237 0.177 , 0.237	Depositor DCC
R_{free} test set	3496 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15062	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1982e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.34	0/3395	0.59	0/4617
1	C	0.33	0/3395	0.58	0/4617
2	B	0.33	0/3794	0.61	1/5145 (0.0%)
2	D	0.33	0/3794	0.60	0/5145
All	All	0.33	0/14378	0.60	1/19524 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	371	GLY	N-CA-C	-5.03	100.54	113.10

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	3320	0	3363	95	0
1	C	3320	0	3363	105	0
2	B	3699	0	3736	141	0
2	D	3699	0	3736	127	0
3	A	239	0	0	7	0
3	B	312	0	0	19	0
3	C	224	0	0	7	0
3	D	249	0	0	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15062	0	14198	438	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 (438) 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:C:32:LYS:HZ2	1:C:32:LYS:N	1.64	0.95
1:C:32:LYS:H	1:C:32:LYS:NZ	1.68	0.91
2:D:12:LYS:HE3	2:D:13:GLY:N	1.85	0.91
1:C:32:LYS:HZ2	1:C:32:LYS:H	0.88	0.88
2:D:235:GLN:HE22	2:D:287:HIS:HE1	1.17	0.88
2:D:367:VAL:CG1	2:D:370:ASP:HB3	2.05	0.86
1:C:97:PRO:HG2	1:C:301:LEU:HD21	1.62	0.82
1:C:65:HIS:HB2	2:D:92:ASP:OD2	1.80	0.81
1:A:335:ALA:HA	2:B:43:PRO:HG2	1.63	0.81
2:D:31:PRO:HB2	2:D:33:GLU:OE2	1.82	0.80
2:B:210:THR:HG22	2:B:239:ASP:HB3	1.64	0.79
1:A:303:LEU:O	1:A:306:ARG:HD3	1.83	0.79
2:B:294:VAL:HG22	2:B:295:PRO:HA	1.65	0.77
2:D:245:ALA:HB2	2:D:375:HIS:HB3	1.68	0.76
1:C:348:LYS:HG3	1:C:419:GLU:HA	1.68	0.75
2:D:12:LYS:HE3	2:D:13:GLY:H	1.52	0.74
1:C:335:ALA:HA	2:D:43:PRO:HG2	1.69	0.74
2:B:68:PHE:HE1	2:B:422:GLU:HG3	1.53	0.73
2:D:235:GLN:HE22	2:D:287:HIS:CE1	2.04	0.73
1:A:66:LYS:HG3	1:A:420:LEU:HD13	1.70	0.72
2:D:30:ILE:HG13	2:D:35:LEU:HD21	1.70	0.72
2:B:442:LYS:NZ	2:B:442:LYS:H	1.87	0.72
1:C:70:GLY:H	1:C:402:THR:HG21	1.54	0.72
2:D:284:VAL:CG2	2:D:288:LEU:HB2	2.19	0.72
2:B:265:HIS:HA	2:B:270:VAL:HB	1.71	0.72
2:B:375:HIS:CE1	2:B:376:GLU:HG2	2.24	0.71
2:D:367:VAL:HG11	2:D:370:ASP:HB3	1.71	0.70
2:B:146:TYR:CE1	2:B:150:ARG:HD2	2.27	0.70
2:B:68:PHE:CE1	2:B:422:GLU:HG3	2.26	0.70
2:D:284:VAL:HG21	2:D:288:LEU:HB2	1.74	0.69
2:D:72:GLY:HA3	2:D:415:MET:HG2	1.73	0.69
2:D:294:VAL:CG2	2:D:308:PHE:HA	2.21	0.69
1:C:268:HIS:O	1:C:326:THR:HG21	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:TYR:HB2	2:D:48:LEU:HG	1.75	0.68
1:A:206:ASN:HD22	1:A:210:ALA:HB3	1.58	0.68
1:C:130:MET:CE	1:C:139:GLU:HG3	2.24	0.68
2:D:73:SER:HA	3:D:532:HOH:O	1.94	0.67
1:C:340:GLU:O	1:C:344:GLU:HG3	1.94	0.66
1:C:269:PHE:HB3	1:C:326:THR:HG23	1.78	0.65
1:C:391:ARG:HH12	2:D:100:ARG:HD3	1.62	0.65
1:A:70:GLY:H	1:A:402:THR:HG21	1.61	0.65
1:C:391:ARG:O	1:C:395:GLU:HG3	1.97	0.65
1:C:396:ARG:CZ	1:C:436:VAL:HG12	2.27	0.65
2:B:4:PRO:HG2	2:B:9:ARG:CZ	2.27	0.64
2:D:85:GLU:HA	2:D:88:ARG:NH1	2.13	0.64
1:A:33:GLU:CD	1:A:33:GLU:H	2.00	0.64
2:B:116:LEU:O	2:B:120:THR:HG22	1.96	0.64
2:B:73:SER:HA	3:B:490:HOH:O	1.97	0.64
2:D:265:HIS:HA	2:D:270:VAL:HB	1.79	0.64
2:D:355:TYR:O	2:D:359:LEU:HD13	1.98	0.64
1:A:97:PRO:HB2	1:A:107:LEU:HD21	1.79	0.64
1:A:396:ARG:HH11	1:A:396:ARG:HG3	1.63	0.64
2:B:85:GLU:HG3	3:B:702:HOH:O	1.98	0.63
1:C:391:ARG:NH1	2:D:100:ARG:HD3	2.14	0.63
1:C:391:ARG:HG3	1:C:391:ARG:HH11	1.63	0.63
1:A:314:LYS:N	1:A:314:LYS:HE3	2.13	0.63
2:B:160:LEU:HD13	2:B:183:ILE:HD11	1.81	0.63
2:B:468:LEU:HD22	2:B:468:LEU:N	2.14	0.63
1:C:130:MET:HE1	1:C:139:GLU:HG3	1.81	0.63
1:C:171:LEU:HD23	1:C:178:LEU:HB2	1.81	0.62
2:D:294:VAL:CG2	2:D:295:PRO:HA	2.29	0.62
2:B:188:GLU:HB2	3:B:496:HOH:O	1.99	0.62
2:D:157:ARG:O	2:D:157:ARG:HG3	1.99	0.62
2:B:387:ALA:H	2:B:412:GLU:HG3	1.65	0.62
1:C:309:TYR:O	1:C:312:ARG:HG2	1.99	0.62
2:B:252:PRO:HA	2:B:255:MET:CE	2.30	0.61
2:B:4:PRO:HG2	2:B:9:ARG:NH2	2.15	0.61
2:D:157:ARG:HH11	2:D:157:ARG:HB2	1.65	0.61
2:B:146:TYR:CZ	2:B:150:ARG:HD2	2.34	0.61
1:A:188:THR:HG22	1:A:212:GLU:OE2	1.99	0.61
1:A:97:PRO:HB2	1:A:107:LEU:CD2	2.30	0.61
1:C:66:LYS:HG2	1:C:420:LEU:HD13	1.81	0.60
2:D:162:PRO:HG2	2:D:165:ALA:HB2	1.83	0.60
1:C:107:LEU:HD11	1:C:301:LEU:HD22	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:LYS:HZ1	2:B:27:GLU:H	1.50	0.60
2:D:367:VAL:HG12	2:D:370:ASP:HB3	1.84	0.60
1:A:359:LEU:HB3	1:A:430:ARG:HD3	1.84	0.60
1:A:1:MET:H1	1:A:1:MET:HE2	1.67	0.59
2:B:367:VAL:CG1	2:B:370:ASP:HB3	2.33	0.59
1:C:233:ASP:O	1:C:237:LEU:HD22	2.01	0.59
1:A:234:PRO:HA	1:A:237:LEU:HD23	1.82	0.59
1:C:143:LEU:HD22	1:C:250:ILE:HD11	1.84	0.59
2:B:23:VAL:HG12	3:B:621:HOH:O	2.02	0.59
2:B:85:GLU:OE2	2:B:88:ARG:HD3	2.02	0.59
2:D:106:LEU:HD11	2:D:306:LEU:HD21	1.85	0.59
2:D:142:ILE:HG23	2:D:291:TYR:HB2	1.85	0.58
2:B:358:GLU:O	2:B:362:GLU:HG3	2.03	0.58
1:A:233:ASP:O	1:A:237:LEU:HD22	2.04	0.58
2:D:403:THR:HB	2:D:415:MET:HB3	1.85	0.58
1:C:234:PRO:HA	1:C:237:LEU:HD23	1.85	0.58
1:A:45:LEU:HD22	1:A:49:LYS:HG2	1.85	0.58
2:B:85:GLU:O	2:B:88:ARG:HG2	2.03	0.58
1:A:32:LYS:N	1:A:32:LYS:HD3	2.19	0.58
2:B:367:VAL:HG12	2:B:370:ASP:HB3	1.86	0.58
2:D:134:HIS:HE1	2:D:318:ARG:HB3	1.70	0.57
2:B:80:PRO:HG2	2:B:83:HIS:CE1	2.39	0.57
2:B:238:TYR:HD2	2:B:260:VAL:HG13	1.70	0.57
2:B:30:ILE:HB	2:B:35:LEU:HD21	1.86	0.57
1:C:431:GLU:OE1	1:C:431:GLU:HA	2.05	0.57
1:A:377:GLU:HG2	1:A:416:ALA:HB2	1.85	0.57
2:B:284:VAL:HG13	2:B:285:LYS:O	2.05	0.57
1:C:241:LYS:HG2	3:D:629:HOH:O	2.04	0.57
2:B:25:LYS:HE3	2:B:27:GLU:H	1.69	0.57
1:C:324:GLN:HG3	2:D:274:GLY:O	2.04	0.57
2:B:424:LYS:O	2:B:428:GLU:HG3	2.05	0.57
1:A:285:ARG:NH2	1:A:321:THR:OG1	2.38	0.56
2:B:403:THR:HB	2:B:415:MET:HB3	1.86	0.56
2:D:157:ARG:NH1	2:D:157:ARG:HB2	2.20	0.56
1:A:66:LYS:HE3	1:A:420:LEU:O	2.05	0.56
1:C:108:GLN:O	1:C:112:GLU:HG3	2.05	0.56
2:D:243:LEU:HD12	2:D:262:LEU:HD22	1.87	0.56
2:D:236:LEU:HD22	2:D:257:PHE:CD2	2.40	0.56
2:B:117:LYS:HA	2:B:120:THR:HG22	1.87	0.56
1:C:128:ALA:O	1:C:129:SER:CB	2.53	0.56
2:B:370:ASP:HA	3:B:590:HOH:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ARG:NE	1:C:376:ASN:HD21	2.04	0.56
1:A:288:SER:HB2	1:A:302:THR:HG21	1.86	0.55
2:B:406:PHE:CD1	2:B:407:PRO:HA	2.40	0.55
2:D:294:VAL:HG21	2:D:308:PHE:HA	1.86	0.55
1:C:318:ASN:HB3	3:C:649:HOH:O	2.06	0.55
1:C:111:PHE:O	1:C:115:THR:HG23	2.05	0.55
2:D:73:SER:HB3	3:D:659:HOH:O	2.06	0.55
1:C:144:ALA:HA	1:C:227:LEU:HD12	1.89	0.55
2:D:211:ASN:HA	2:D:212:PRO:C	2.27	0.55
2:D:4:PRO:HG2	2:D:9:ARG:CZ	2.36	0.55
2:B:25:LYS:CE	2:B:27:GLU:H	2.20	0.55
1:A:391:ARG:O	1:A:395:GLU:HG3	2.08	0.54
2:D:4:PRO:HG2	2:D:9:ARG:NH2	2.23	0.54
1:A:108:GLN:O	1:A:112:GLU:HG3	2.08	0.54
1:C:185:GLY:O	1:C:371:PRO:HG3	2.07	0.54
2:D:117:LYS:HD2	2:D:125:ILE:HG22	1.90	0.54
1:C:128:ALA:O	1:C:129:SER:HB3	2.06	0.54
2:D:102:ALA:O	2:D:106:LEU:HD22	2.07	0.54
2:D:170:PRO:HB3	2:D:180:VAL:HG21	1.89	0.54
1:C:143:LEU:HD23	1:C:143:LEU:C	2.28	0.54
2:D:269:THR:HA	3:D:553:HOH:O	2.08	0.54
2:B:25:LYS:HE2	2:B:27:GLU:OE1	2.07	0.54
1:C:346:ALA:O	1:C:350:VAL:HG23	2.08	0.54
2:B:10:SER:HB2	2:B:44:GLU:H	1.73	0.53
2:B:120:THR:HG23	2:B:122:MET:H	1.73	0.53
2:B:289:ALA:N	2:B:290:PRO:HD2	2.23	0.53
1:C:143:LEU:HD23	1:C:143:LEU:O	2.08	0.53
2:D:406:PHE:CD1	2:D:407:PRO:HA	2.44	0.53
2:B:252:PRO:HA	2:B:255:MET:HE2	1.91	0.53
2:B:337:LEU:HB3	2:B:341:GLY:HA3	1.89	0.53
1:C:309:TYR:HD1	1:C:312:ARG:HH11	1.56	0.53
1:A:396:ARG:HG3	1:A:396:ARG:NH1	2.23	0.53
2:B:25:LYS:NZ	2:B:27:GLU:H	2.06	0.53
2:B:471:PHE:O	2:B:472:ASP:C	2.46	0.53
2:D:138:THR:O	2:D:142:ILE:HG13	2.08	0.53
1:A:4:THR:HG21	2:B:348:LEU:HD12	1.91	0.53
1:C:239:VAL:HG21	1:C:347:LEU:HD21	1.90	0.53
2:B:91:ALA:HB2	3:B:775:HOH:O	2.08	0.53
2:D:363:LYS:HG2	2:D:435:GLY:HA3	1.90	0.53
2:B:386:ARG:NH2	2:B:388:LEU:HD23	2.24	0.53
2:D:203:HIS:H	2:D:203:HIS:CD2	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:THR:HG22	2:D:469:THR:HA	1.91	0.53
2:B:236:LEU:HG	2:B:257:PHE:CD1	2.44	0.53
2:B:468:LEU:H	2:B:468:LEU:HD22	1.74	0.53
1:C:316:LYS:HG2	3:D:575:HOH:O	2.09	0.53
2:D:144:ARG:NH2	2:D:176:ALA:O	2.40	0.53
2:B:442:LYS:H	2:B:442:LYS:CE	2.22	0.52
2:D:166:HIS:HA	2:D:406:PHE:CZ	2.43	0.52
1:A:9:GLU:CD	1:A:9:GLU:H	2.11	0.52
2:D:33:GLU:CD	2:D:33:GLU:H	2.12	0.52
2:B:134:HIS:CE1	2:B:318:ARG:HB3	2.44	0.52
1:C:314:LYS:HE3	1:C:314:LYS:N	2.24	0.52
2:D:68:PHE:CE1	2:D:422:GLU:HG3	2.44	0.52
2:B:134:HIS:HE1	2:B:318:ARG:HB3	1.75	0.52
1:C:285:ARG:HG3	1:C:285:ARG:HH11	1.73	0.52
1:C:95:TYR:CG	1:C:96:THR:N	2.78	0.52
3:A:499:HOH:O	2:B:468:LEU:HB3	2.10	0.52
2:B:252:PRO:HA	2:B:255:MET:HE3	1.92	0.52
2:D:284:VAL:HG22	2:D:288:LEU:HB2	1.89	0.52
2:D:359:LEU:O	2:D:362:GLU:HB2	2.09	0.52
1:A:255:GLY:HA3	1:A:269:PHE:CE2	2.45	0.52
1:A:280:ARG:HD2	1:A:309:TYR:CE2	2.45	0.52
2:B:181:ARG:NH1	2:B:199:GLU:OE2	2.43	0.52
2:B:163:ASP:OD2	2:B:184:PRO:HA	2.10	0.52
2:D:238:TYR:HB2	2:D:257:PHE:CD2	2.45	0.52
2:B:69:TYR:CD1	2:B:71:LEU:HD22	2.45	0.51
2:B:238:TYR:HB2	2:B:257:PHE:CD1	2.45	0.51
2:B:33:GLU:HB3	3:B:726:HOH:O	2.10	0.51
2:B:441:PRO:HG2	2:B:444:TRP:HB2	1.92	0.51
1:C:196:GLU:HA	3:C:659:HOH:O	2.10	0.51
1:C:319:ILE:HA	3:C:465:HOH:O	2.10	0.51
2:B:48:LEU:HG	2:D:78:TYR:HB2	1.92	0.51
2:D:235:GLN:NE2	2:D:287:HIS:HE1	1.98	0.51
1:A:309:TYR:HD1	1:A:312:ARG:HH11	1.57	0.51
1:C:391:ARG:HG3	1:C:391:ARG:NH1	2.26	0.51
2:B:146:TYR:O	2:B:150:ARG:HG3	2.11	0.51
1:C:313:ALA:C	1:C:314:LYS:HE3	2.31	0.51
2:D:210:THR:HG22	2:D:239:ASP:HB3	1.91	0.51
1:A:402:THR:HG23	1:A:414:LEU:CB	2.41	0.51
1:A:115:THR:HB	2:B:469:THR:HB	1.92	0.51
1:C:402:THR:HG23	1:C:414:LEU:HB2	1.92	0.51
2:D:134:HIS:CE1	2:D:318:ARG:HB3	2.47	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:472:ASP:HA	3:D:636:HOH:O	2.11	0.51
1:C:168:ARG:O	1:C:172:GLU:HG3	2.11	0.50
1:A:241:LYS:HD3	1:A:246:TYR:CE1	2.46	0.50
2:B:381:PRO:HB3	2:B:390:LEU:CD1	2.41	0.50
2:D:242:ASN:HB3	2:D:375:HIS:CE1	2.47	0.50
1:A:32:LYS:H	1:A:32:LYS:HZ2	1.58	0.50
2:D:195:ALA:HA	2:D:198:ARG:CZ	2.42	0.50
1:A:95:TYR:HD1	2:B:272:HIS:HB3	1.76	0.50
1:A:95:TYR:CD1	2:B:272:HIS:HB3	2.47	0.50
2:B:357:LYS:NZ	2:B:370:ASP:HB2	2.26	0.50
2:B:442:LYS:H	2:B:442:LYS:HZ3	1.58	0.50
2:B:368:PRO:HG2	3:B:503:HOH:O	2.11	0.50
2:D:69:TYR:HB3	2:D:76:MET:HG3	1.93	0.50
1:A:293:VAL:HG13	1:A:294:GLU:HG3	1.93	0.49
1:A:292:ASP:HB3	2:B:454:VAL:HG22	1.94	0.49
1:C:106:VAL:HG23	2:D:61:GLN:CD	2.33	0.49
1:A:267:PRO:HD3	2:B:325:LEU:HD22	1.93	0.49
1:C:309:TYR:HD1	1:C:312:ARG:NH1	2.10	0.49
1:C:51:LEU:HG	2:D:82:LEU:HD11	1.94	0.49
1:C:168:ARG:HD3	3:C:651:HOH:O	2.12	0.49
2:D:318:ARG:HD3	2:D:319:SER:O	2.12	0.49
2:D:294:VAL:HG22	2:D:295:PRO:HA	1.93	0.49
1:C:64:ALA:O	1:C:67:ALA:HB2	2.11	0.49
2:B:394:LEU:HD23	2:B:401:PRO:HA	1.95	0.49
2:B:459:GLU:HG3	3:B:695:HOH:O	2.12	0.49
2:B:69:TYR:HD1	2:B:71:LEU:HD22	1.78	0.49
2:B:294:VAL:CG2	2:B:308:PHE:HA	2.43	0.49
1:C:45:LEU:HD22	1:C:49:LYS:HG2	1.94	0.49
2:D:181:ARG:NH1	2:D:199:GLU:OE1	2.46	0.49
2:B:169:ASN:HB2	2:B:170:PRO:CD	2.43	0.49
1:C:4:THR:HG21	2:D:344:LYS:HE2	1.95	0.48
2:D:236:LEU:HD22	2:D:257:PHE:CE2	2.48	0.48
1:C:402:THR:HG23	1:C:414:LEU:O	2.13	0.48
2:D:394:LEU:HD13	2:D:437:LEU:HD11	1.94	0.48
2:B:359:LEU:O	2:B:363:LYS:HG2	2.13	0.48
1:C:280:ARG:HD2	1:C:309:TYR:CE2	2.47	0.48
2:D:129:PRO:HG2	2:D:280:GLY:O	2.14	0.48
2:D:154:ARG:HH11	2:D:154:ARG:HG3	1.79	0.48
2:D:289:ALA:N	2:D:290:PRO:HD2	2.29	0.48
2:D:236:LEU:HB3	2:D:257:PHE:HA	1.96	0.48
1:A:32:LYS:HD3	1:A:32:LYS:H	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:HG2	2:D:318:ARG:HG3	1.94	0.48
2:D:456:ARG:HG3	3:D:510:HOH:O	2.14	0.48
1:A:32:LYS:NZ	1:A:32:LYS:H	2.12	0.48
1:A:42:PRO:HG2	3:A:449:HOH:O	2.13	0.48
1:C:201:VAL:HG22	1:C:229:VAL:HB	1.96	0.48
1:C:377:GLU:HG2	1:C:416:ALA:HB2	1.96	0.48
2:B:181:ARG:HG2	2:B:181:ARG:HH11	1.79	0.48
2:D:441:PRO:HG2	2:D:444:TRP:HB2	1.96	0.48
1:A:139:GLU:CD	1:A:319:ILE:HD11	2.35	0.47
2:D:128:GLU:N	2:D:129:PRO:HD2	2.28	0.47
2:D:370:ASP:HA	3:D:675:HOH:O	2.14	0.47
1:A:402:THR:HG23	1:A:414:LEU:HB2	1.95	0.47
2:B:294:VAL:CG2	2:B:295:PRO:HA	2.40	0.47
2:D:284:VAL:HG21	2:D:288:LEU:CB	2.43	0.47
2:B:31:PRO:HG2	2:B:34:HIS:HD2	1.78	0.47
2:D:363:LYS:N	2:D:363:LYS:HD2	2.29	0.47
2:D:402:PRO:HB2	2:D:415:MET:O	2.15	0.47
2:B:210:THR:OG1	2:B:213:ASN:HA	2.14	0.47
1:A:171:LEU:HD23	1:A:178:LEU:HB2	1.97	0.47
2:B:73:SER:HB3	2:B:415:MET:CE	2.44	0.47
1:C:306:ARG:O	1:C:310:ILE:HG13	2.13	0.47
1:A:128:ALA:O	1:A:129:SER:CB	2.62	0.47
1:A:352:MET:HE3	1:A:426:LEU:HD11	1.97	0.47
1:C:154:LEU:HD22	1:C:179:LEU:HD23	1.96	0.47
2:D:131:ALA:HB2	2:D:278:GLY:HA3	1.97	0.47
2:D:235:GLN:HE21	2:D:288:LEU:HD11	1.80	0.47
1:A:188:THR:O	1:A:217:PHE:HZ	1.98	0.47
2:D:245:ALA:HB2	2:D:375:HIS:CB	2.40	0.47
2:D:120:THR:HA	2:D:252:PRO:HD2	1.97	0.47
2:B:395:LEU:HD13	2:B:401:PRO:HD3	1.95	0.47
2:B:242:ASN:HB3	2:B:375:HIS:CE1	2.50	0.47
2:D:381:PRO:HB3	2:D:390:LEU:CD1	2.46	0.47
2:B:291:TYR:O	2:B:314:ILE:HG23	2.16	0.46
1:A:74:ARG:NE	1:A:376:ASN:HD21	2.13	0.46
2:B:267:THR:HB	2:B:268:PHE:CD1	2.50	0.46
2:B:395:LEU:CD1	2:B:401:PRO:HD3	2.44	0.46
2:D:394:LEU:HD13	2:D:437:LEU:CD1	2.45	0.46
2:D:87:ALA:HB1	2:D:325:LEU:HG	1.97	0.46
1:A:7:THR:OG1	1:A:9:GLU:HG2	2.16	0.46
1:C:323:ALA:HB1	1:C:326:THR:CG2	2.45	0.46
2:D:85:GLU:HA	2:D:88:ARG:HH11	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:O	1:A:267:PRO:HG2	2.16	0.46
2:D:80:PRO:HG2	2:D:83:HIS:CE1	2.51	0.46
1:C:319:ILE:HG23	1:C:319:ILE:O	2.16	0.46
2:D:136:GLU:OE2	2:D:169:ASN:ND2	2.47	0.46
2:D:262:LEU:O	2:D:280:GLY:HA2	2.15	0.46
1:A:56:ARG:HH22	2:B:107:ARG:NH1	2.14	0.46
1:C:130:MET:HE2	1:C:139:GLU:HG3	1.97	0.46
3:B:576:HOH:O	1:C:1:MET:HG3	2.16	0.46
1:A:377:GLU:HG2	1:A:416:ALA:CB	2.45	0.46
2:D:294:VAL:HG22	2:D:295:PRO:CA	2.46	0.46
2:B:267:THR:HB	2:B:268:PHE:CE1	2.51	0.46
1:A:373:PRO:HG3	2:B:31:PRO:HG3	1.98	0.46
1:C:97:PRO:HG3	1:C:107:LEU:HD13	1.97	0.45
1:C:280:ARG:HD3	3:C:591:HOH:O	2.16	0.45
1:C:32:LYS:HD3	1:C:32:LYS:N	2.31	0.45
2:D:68:PHE:HE1	2:D:422:GLU:HG3	1.80	0.45
2:B:107:ARG:O	2:B:111:GLU:HG3	2.16	0.45
1:A:311:ARG:HA	1:A:316:LYS:HG2	1.99	0.45
1:C:115:THR:CG2	2:D:470:TYR:H	2.30	0.45
2:D:301:GLU:HG3	3:D:723:HOH:O	2.15	0.45
2:B:88:ARG:HA	3:B:775:HOH:O	2.15	0.45
1:C:364:PRO:HG2	3:C:495:HOH:O	2.16	0.45
1:A:337:LEU:HD13	2:B:17:LEU:HB2	1.99	0.45
1:A:74:ARG:CZ	1:A:376:ASN:HD21	2.29	0.45
1:A:422:GLU:OE2	1:C:49:LYS:NZ	2.36	0.45
2:B:25:LYS:HE3	2:B:27:GLU:N	2.31	0.45
1:C:433:LEU:HG	1:C:437:LEU:HD22	1.99	0.45
2:B:318:ARG:HD3	2:B:319:SER:O	2.17	0.45
2:B:411:LYS:HD3	2:B:412:GLU:HB2	1.98	0.45
1:A:284:GLY:O	1:A:306:ARG:NH2	2.47	0.45
2:B:10:SER:CB	2:B:44:GLU:H	2.30	0.45
1:A:360:LEU:HD12	1:A:430:ARG:HG3	1.98	0.44
1:A:79:PRO:HA	1:A:80:PRO:HD2	1.85	0.44
2:D:107:ARG:O	2:D:111:GLU:HG3	2.16	0.44
1:A:146:ARG:HD3	1:A:315:ALA:O	2.17	0.44
2:B:72:GLY:HA2	2:B:417:GLU:HB2	1.98	0.44
2:D:183:ILE:HG22	2:D:199:GLU:HG3	2.00	0.44
1:A:8:GLU:O	1:A:12:ARG:HG3	2.18	0.44
2:B:157:ARG:HB3	3:B:732:HOH:O	2.17	0.44
2:B:381:PRO:HG2	3:B:597:HOH:O	2.17	0.44
1:C:404:VAL:HG22	1:C:414:LEU:HG	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:CG	1:A:96:THR:N	2.85	0.44
3:A:504:HOH:O	2:B:175:MET:HE2	2.16	0.44
1:A:286:LEU:HD22	2:B:468:LEU:HD12	1.99	0.44
1:C:348:LYS:HE3	2:D:20:VAL:HG13	1.99	0.44
2:D:31:PRO:HG2	2:D:34:HIS:HD2	1.83	0.44
1:A:23:LEU:HG	2:B:347:ALA:HB1	1.98	0.44
2:B:73:SER:HB3	2:B:415:MET:HE2	1.98	0.44
1:C:285:ARG:NH1	1:C:285:ARG:HG3	2.33	0.44
2:D:77:LYS:HD2	2:D:269:THR:HG22	1.98	0.44
1:C:158:GLY:HA3	1:C:206:ASN:OD1	2.18	0.44
1:A:144:ALA:HA	1:A:227:LEU:HD12	2.00	0.44
1:A:222:HIS:HE1	1:A:249:ASP:OD2	2.01	0.44
2:D:203:HIS:H	2:D:203:HIS:HD2	1.64	0.44
2:B:284:VAL:HG22	2:B:288:LEU:HB2	2.00	0.43
2:B:106:LEU:HD21	2:B:306:LEU:HD21	1.99	0.43
1:C:222:HIS:HE1	1:C:249:ASP:OD2	2.01	0.43
1:C:269:PHE:HB3	1:C:326:THR:CG2	2.46	0.43
2:D:294:VAL:HG23	2:D:295:PRO:HA	1.99	0.43
2:B:181:ARG:HD2	3:B:542:HOH:O	2.17	0.43
3:A:452:HOH:O	2:B:453:PRO:HG2	2.17	0.43
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.90	0.43
1:A:271:PHE:CD1	1:A:271:PHE:C	2.91	0.43
1:C:260:LEU:HD21	1:C:326:THR:OG1	2.19	0.43
2:B:440:LYS:HG2	2:B:444:TRP:CE3	2.54	0.43
1:A:137:LEU:HD11	1:A:201:VAL:HG11	2.00	0.43
1:A:1:MET:HG3	3:A:535:HOH:O	2.19	0.43
1:A:292:ASP:HB3	2:B:454:VAL:CG2	2.49	0.43
1:A:346:ALA:O	1:A:350:VAL:HG23	2.18	0.43
1:C:286:LEU:HB2	1:C:306:ARG:NH2	2.34	0.43
2:D:237:TYR:CD1	2:D:237:TYR:C	2.92	0.43
1:A:1:MET:N	1:A:1:MET:HE2	2.31	0.43
2:B:129:PRO:HG2	2:B:280:GLY:O	2.18	0.43
2:B:179:GLN:NE2	3:B:593:HOH:O	2.51	0.43
1:A:15:LEU:HD13	1:A:22:SER:HA	2.01	0.43
2:D:210:THR:OG1	2:D:213:ASN:HA	2.19	0.43
2:D:323:ASN:O	2:D:327:LEU:HG	2.19	0.43
2:B:455:ARG:HB3	3:B:595:HOH:O	2.18	0.43
2:B:81:LYS:HE3	3:B:545:HOH:O	2.18	0.43
2:D:206:ALA:HA	2:D:234:VAL:HG13	2.01	0.43
2:D:397:LEU:HD23	2:D:433:ALA:HB1	2.00	0.43
1:C:115:THR:HB	2:D:469:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:PRO:HA	1:C:237:LEU:CD2	2.49	0.42
1:A:261:PRO:O	1:A:267:PRO:CG	2.67	0.42
1:A:348:LYS:HE2	3:A:511:HOH:O	2.19	0.42
2:B:83:HIS:CE1	2:B:333:TYR:HB2	2.54	0.42
2:D:212:PRO:CG	2:D:374:MET:HG3	2.49	0.42
1:A:115:THR:O	1:A:119:GLU:HG2	2.18	0.42
1:A:143:LEU:CD2	1:A:281:GLN:HB3	2.48	0.42
2:B:181:ARG:HG2	2:B:181:ARG:NH1	2.33	0.42
2:B:264:LEU:HD22	2:B:279:SER:OG	2.19	0.42
1:C:206:ASN:HD22	1:C:210:ALA:HB3	1.84	0.42
2:B:211:ASN:HA	2:B:212:PRO:C	2.39	0.42
2:B:381:PRO:HB3	2:B:390:LEU:HD11	2.02	0.42
1:C:128:ALA:HB3	1:C:285:ARG:HB2	2.01	0.42
1:A:386:PRO:HD3	1:A:411:ASN:HA	2.01	0.42
2:B:120:THR:HA	2:B:252:PRO:HD2	2.01	0.42
1:C:282:LEU:HD12	1:C:283:PRO:HD2	2.02	0.42
1:C:357:HIS:HB2	1:C:378:PHE:CE2	2.55	0.42
2:D:238:TYR:CE2	2:D:240:GLY:HA2	2.55	0.42
2:B:138:THR:O	2:B:142:ILE:HG13	2.20	0.42
1:C:17:ARG:HG3	1:C:17:ARG:HH11	1.84	0.42
1:A:7:THR:OG1	1:A:10:GLU:HG3	2.18	0.42
2:B:382:PRO:HG2	2:B:385:PHE:CD1	2.54	0.42
2:B:394:LEU:HD12	2:B:394:LEU:HA	1.89	0.42
2:B:128:GLU:N	2:B:129:PRO:HD2	2.35	0.42
2:B:210:THR:CG2	2:B:239:ASP:HB3	2.43	0.42
2:B:77:LYS:HD2	2:B:269:THR:HG22	2.01	0.42
1:C:316:LYS:HD3	3:D:673:HOH:O	2.19	0.42
1:A:9:GLU:O	1:A:13:GLU:HG3	2.20	0.42
1:C:1:MET:H1	1:C:1:MET:CE	2.33	0.42
2:D:86:ALA:O	2:D:89:LEU:HB2	2.19	0.42
1:A:308:GLN:N	1:A:308:GLN:HE21	2.18	0.41
2:B:117:LYS:HA	2:B:120:THR:CG2	2.48	0.41
2:D:363:LYS:HG2	2:D:435:GLY:CA	2.50	0.41
2:B:213:ASN:HB2	3:B:553:HOH:O	2.20	0.41
2:B:294:VAL:HG22	2:B:308:PHE:HA	2.02	0.41
1:A:132:ASP:OD1	1:A:135:THR:HG23	2.20	0.41
1:A:355:LYS:HG3	3:A:601:HOH:O	2.20	0.41
1:C:367:ARG:HG3	1:C:368:PRO:HD2	2.01	0.41
2:D:397:LEU:HD22	2:D:437:LEU:HD21	2.03	0.41
1:A:393:LEU:HD13	1:A:436:VAL:HG21	2.00	0.41
2:B:158:VAL:O	2:B:205:ALA:N	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:ALA:HB3	2:B:374:MET:O	2.20	0.41
2:B:410:VAL:O	2:B:413:ALA:HB2	2.21	0.41
2:B:454:VAL:HG21	2:B:457:LEU:HD21	2.03	0.41
1:C:301:LEU:HD23	3:C:445:HOH:O	2.21	0.41
2:D:245:ALA:HB2	2:D:375:HIS:CG	2.56	0.41
1:A:286:LEU:HB2	1:A:306:ARG:NH1	2.36	0.41
2:B:262:LEU:O	2:B:280:GLY:HA2	2.20	0.41
1:C:115:THR:HG21	2:D:470:TYR:H	1.85	0.41
1:C:150:ARG:HD3	1:C:195:GLU:O	2.21	0.41
1:C:281:GLN:OE1	1:C:310:ILE:HA	2.21	0.41
2:D:146:TYR:CE1	2:D:150:ARG:HD2	2.55	0.41
2:D:210:THR:CG2	2:D:239:ASP:HB3	2.50	0.41
2:D:354:ARG:HG2	2:D:373:SER:HB2	2.03	0.41
2:B:386:ARG:HH21	2:B:388:LEU:HD23	1.86	0.41
1:C:291:VAL:CG1	1:C:295:GLY:HA2	2.51	0.41
1:C:348:LYS:CG	1:C:419:GLU:HA	2.45	0.41
1:C:50:VAL:O	1:C:54:LEU:HD22	2.21	0.41
1:A:32:LYS:H	1:A:32:LYS:CD	2.34	0.41
1:A:32:LYS:HZ3	1:A:32:LYS:HB2	1.86	0.41
1:A:347:LEU:HB3	2:B:24:PRO:HG2	2.02	0.41
1:C:184:GLU:OE2	1:C:189:PRO:HG3	2.20	0.41
1:C:130:MET:HE3	1:C:319:ILE:HD12	2.02	0.41
2:D:108:LEU:C	2:D:108:LEU:HD23	2.41	0.41
2:D:224:GLU:HB2	3:D:717:HOH:O	2.20	0.41
1:A:420:LEU:C	1:A:420:LEU:HD12	2.41	0.40
2:B:122:MET:HG3	2:B:283:GLY:HA3	2.03	0.40
1:A:203:GLN:HG2	1:A:205:PRO:O	2.21	0.40
2:D:310:ARG:HH11	2:D:310:ARG:HG2	1.86	0.40
2:D:68:PHE:CZ	2:D:70:PRO:HB3	2.56	0.40
1:A:281:GLN:HA	1:A:281:GLN:OE1	2.21	0.40
1:A:385:ASP:O	1:A:389:VAL:HG23	2.21	0.40
2:B:232:ALA:HB2	3:B:758:HOH:O	2.21	0.40
1:C:234:PRO:HG3	1:C:255:GLY:HA2	2.04	0.40
1:A:97:PRO:HB2	1:A:107:LEU:HD22	2.02	0.40
1:C:402:THR:CG2	1:C:414:LEU:O	2.70	0.40
2:D:169:ASN:HB2	2:D:170:PRO:CD	2.51	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	435/438 (99%)	415 (95%)	19 (4%)	1 (0%)	47 62
1	C	435/438 (99%)	416 (96%)	17 (4%)	2 (0%)	29 41
2	B	469/474 (99%)	451 (96%)	18 (4%)	0	100 100
2	D	469/474 (99%)	445 (95%)	24 (5%)	0	100 100
All	All	1808/1824 (99%)	1727 (96%)	78 (4%)	3 (0%)	47 62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	129	SER
1	A	129	SER
1	C	313	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	336/336 (100%)	319 (95%)	17 (5%)	24 39
1	C	336/336 (100%)	315 (94%)	21 (6%)	18 28
2	B	383/385 (100%)	358 (94%)	25 (6%)	17 27
2	D	383/385 (100%)	358 (94%)	25 (6%)	17 27
All	All	1438/1442 (100%)	1350 (94%)	88 (6%)	18 30

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	32	LYS
1	A	41	LEU
1	A	107	LEU
1	A	115	THR
1	A	171	LEU
1	A	188	THR
1	A	237	LEU
1	A	280	ARG
1	A	307	GLU
1	A	308	GLN
1	A	314	LYS
1	A	334	LEU
1	A	360	LEU
1	A	393	LEU
1	A	402	THR
1	A	427	LEU
2	B	25	LYS
2	B	42	LEU
2	B	48	LEU
2	B	69	TYR
2	B	71	LEU
2	B	81	LYS
2	B	89	LEU
2	B	141	LEU
2	B	148	GLU
2	B	181	ARG
2	B	243	LEU
2	B	259	VAL
2	B	264	LEU
2	B	284	VAL
2	B	294	VAL
2	B	302	GLU
2	B	318	ARG
2	B	325	LEU
2	B	360	LEU
2	B	394	LEU
2	B	395	LEU
2	B	397	LEU
2	B	411	LYS
2	B	432	GLU
2	B	472	ASP
1	C	4	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	32	LYS
1	C	41	LEU
1	C	54	LEU
1	C	107	LEU
1	C	115	THR
1	C	171	LEU
1	C	183	LEU
1	C	237	LEU
1	C	269	PHE
1	C	272	LEU
1	C	275	LYS
1	C	286	LEU
1	C	314	LYS
1	C	324	GLN
1	C	328	LEU
1	C	334	LEU
1	C	393	LEU
1	C	402	THR
1	C	427	LEU
1	C	431	GLU
2	D	12	LYS
2	D	30	ILE
2	D	48	LEU
2	D	71	LEU
2	D	89	LEU
2	D	92	ASP
2	D	100	ARG
2	D	106	LEU
2	D	141	LEU
2	D	148	GLU
2	D	157	ARG
2	D	203	HIS
2	D	214	THR
2	D	236	LEU
2	D	243	LEU
2	D	302	GLU
2	D	318	ARG
2	D	325	LEU
2	D	394	LEU
2	D	395	LEU
2	D	397	LEU
2	D	442	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	445	LEU
2	D	454	VAL
2	D	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	308	GLN
1	A	318	ASN
1	A	354	HIS
2	B	34	HIS
2	B	235	GLN
2	B	380	GLN
2	B	447	ASN
1	C	222	HIS
1	C	376	ASN
2	D	34	HIS
2	D	203	HIS
2	D	235	GLN
2	D	287	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	437/438 (99%)	-0.70	1 (0%) 95 94	17, 27, 44, 74	0
1	C	437/438 (99%)	-0.68	0 100 100	17, 28, 45, 60	0
2	B	471/474 (99%)	-0.74	1 (0%) 95 94	16, 25, 42, 65	0
2	D	471/474 (99%)	-0.75	1 (0%) 95 94	17, 27, 42, 63	0
All	All	1816/1824 (99%)	-0.72	3 (0%) 95 94	16, 27, 43, 74	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ARG	3.1
2	D	443	GLU	2.5
2	B	301	GLU	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.