Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 10:58 pm BST

PDB ID	:	2V0V
Title	:	Crystal Structure of Rev-Erb beta
Authors	:	Woo, E.-J.; Jeong, D.G.; Lim, M.-Y.; Jun Kim, S.; Eon Ryu, S.
Deposited on	:	2007-05-19
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

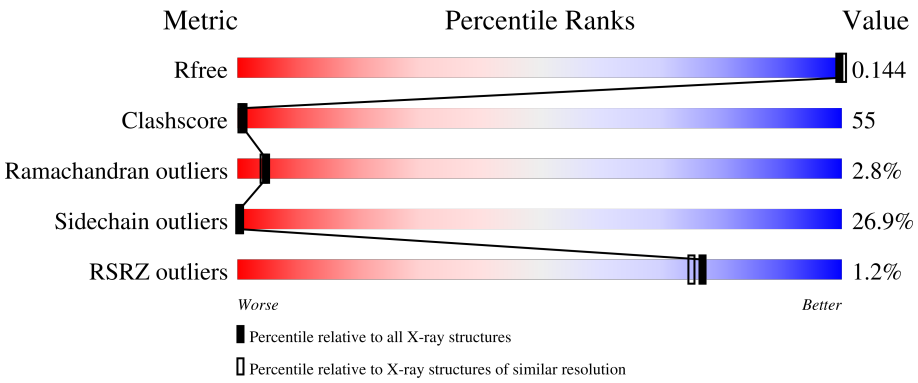
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 of 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	194	.% 26% 51% 14% • 7%
1	B	194	.% 26% 49% 17% • 7%
1	C	194	.% 26% 47% 20% 8%
1	D	194	2% 21% 50% 21% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5810 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 ORPHAN NUCLEAR RECEPTOR NR1D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	181	1436	915	241	273	7	0	0	0
1	B	181	1436	915	241	273	7	0	0	0
1	C	179	1421	906	238	270	7	0	0	0
1	D	179	1421	906	238	270	7	0	0	0

- Molecule 2 is water.

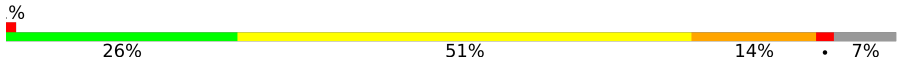
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	23	23	23	0	0
2	B	26	26	26	0	0
2	C	22	22	22	0	0
2	D	25	25	25	0	0

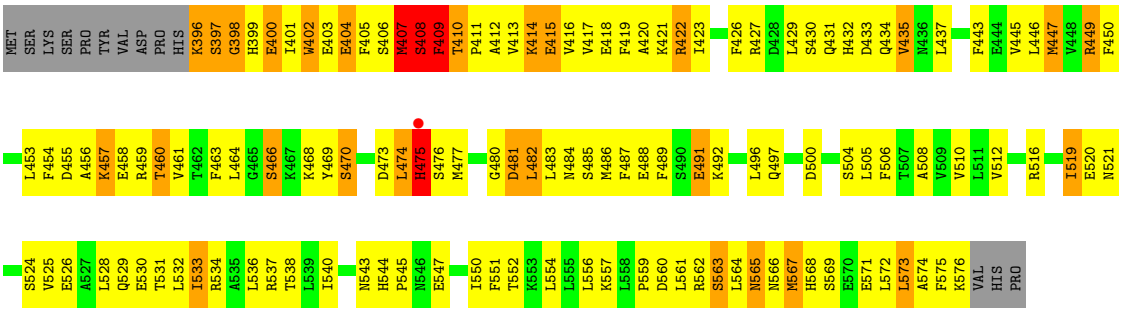
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ORPHAN NUCLEAR RECEPTOR NR1D2

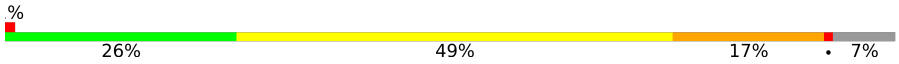
Chain A:

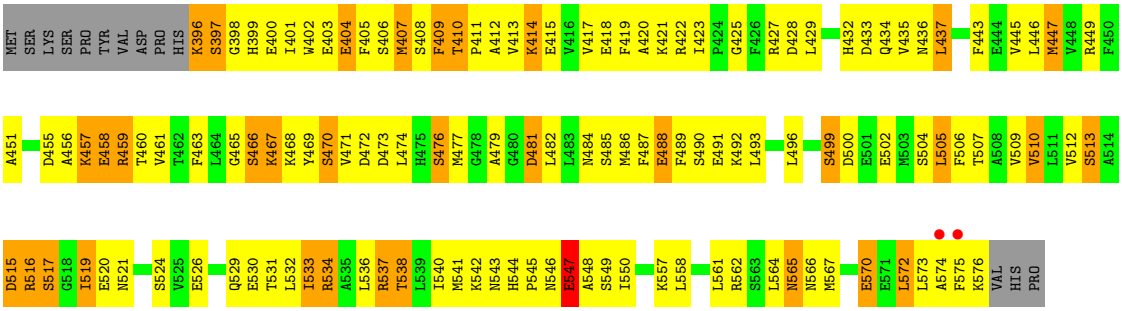




• Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

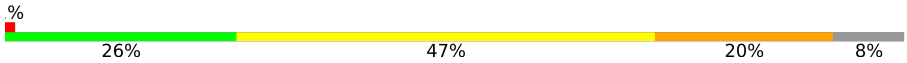
Chain B:

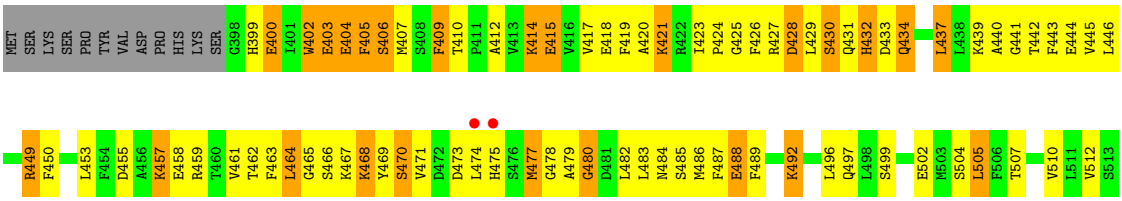


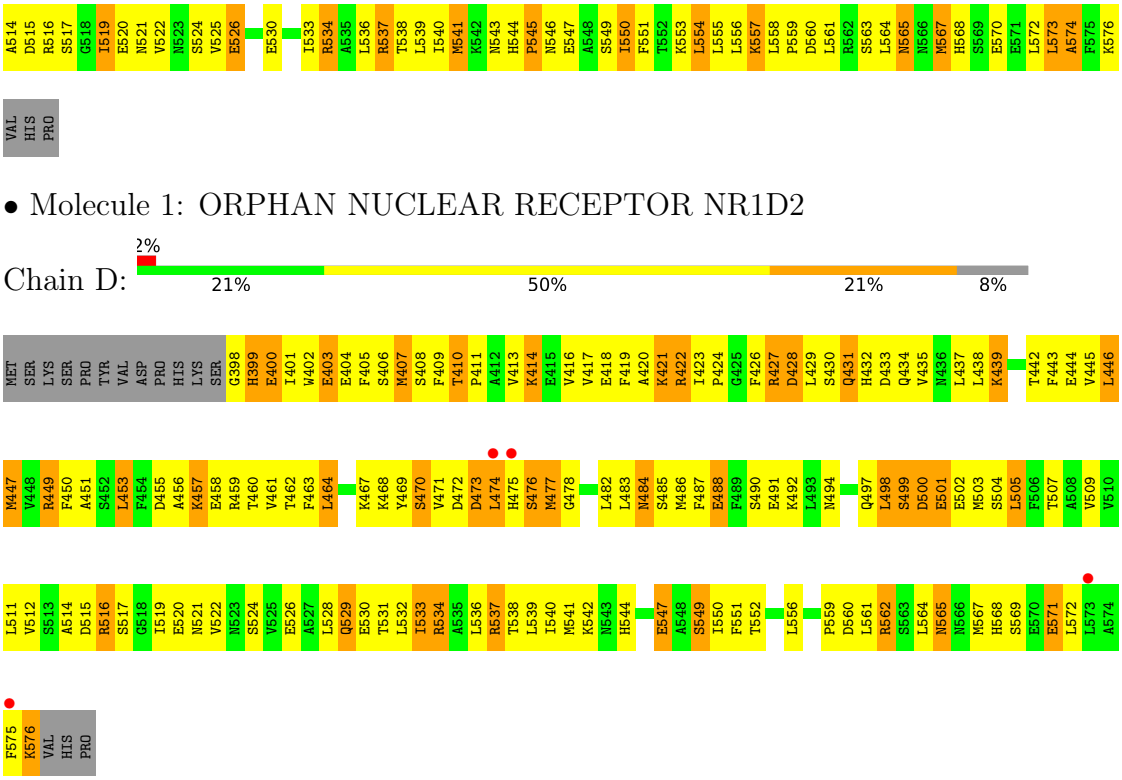


• Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

Chain C:






A514 D515 R516 S517 G518 I519 E520 N521 V522 N523 S524 V525 E526 E530 I533 R534 A535 L536 R537 T538 L539 I540 M541 K542 N543 H544 P545 N546 E547 A548 S549 I550 F551 T552 K553 L554 L555 L556 K557 L558 P559 D560 L561 R562 S563 L564 N565 N566 M567 H568 S569 E570 E571 L572 L573 A574 F575 K576
VAL HIS PRO
• Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2
Chain D:
2%
21%
50%
21%
8%
MET SER LYS SER PRO TYR VAL ASP PRO HIS LYS SER G398 H399 E400 I401 W402 E403 E404 F405 S406 M407 S408 F409 T410 P411 A412 V413 K414 E415 V416 V417 E418 F419 A420 K421 R422 I423 P424 G425 F426 R427 D428 L429 S430 Q431 H432 D433 Q434 V435 N436 L437 L438 K439 T442 F443 E444 V445 L446
M447 V448 R449 F450 A451 S452 L453 F454 D455 A456 K457 E458 R459 T460 V461 T462 F463 L464 K467 K468 Y469 S470 V471 D472 D473 L474 H475 S476 M477 G478 L482 L483 N484 S485 M486 F487 E488 F489 S490 E491 K492 L493 N494 Q497 L498 S499 D500 E501 E502 M503 S504 L505 F506 T507 A508 V509 V510
L511 V512 S513 A514 D515 R516 S517 G518 I519 E520 N521 V522 N523 S524 V525 E526 A527 L528 Q529 E530 T531 L532 I533 R534 A535 L536 R537 T538 L539 I540 M541 K542 N543 H544 E547 A548 S549 I550 F551 T552 L556 P559 D560 L561 R562 S563 L564 N565 N566 M567 H568 S569 E570 E571 L572 L573 A574
F575 K576 VAL HIS PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	102.46Å 102.46Å 143.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.40 29.54 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.6 (99.00-2.40) 90.8 (29.54-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.29Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.138 , 0.220 0.145 , 0.144	Depositor DCC
R_{free} test set	1484 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.096 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.096 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.097 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.096 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.487 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5810	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.33	0/1460	0.97	3/1965 (0.2%)
1	B	0.39	0/1460	0.87	0/1965
1	C	0.33	0/1445	0.90	0/1946
1	D	0.38	0/1445	0.91	1/1946 (0.1%)
All	All	0.36	0/5810	0.91	4/7822 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	SER	CB-CA-C	10.55	130.14	110.10
1	A	409	PHE	N-CA-CB	-5.99	99.82	110.60
1	A	409	PHE	N-CA-C	5.95	127.07	111.00
1	D	562	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	410	THR	Peptide
1	A	475	HIS	Peptide
1	B	476	SER	Peptide
1	B	547	GLU	Peptide
1	C	567	MET	Peptide
1	D	464	LEU	Peptide

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	1436	0	1446	147	0
1	B	1436	0	1446	172	0
1	C	1421	0	1428	163	0
1	D	1421	0	1428	166	0
2	A	23	0	0	3	0
2	B	26	0	0	5	0
2	C	22	0	0	7	0
2	D	25	0	0	10	0
All	All	5810	0	5748	633	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 55.

All (633) 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:473:ASP:C	1:B:477:MET:HG2	1.47	1.33
1:B:473:ASP:O	1:B:477:MET:CG	1.80	1.28
1:A:470:SER:HB3	1:A:473:ASP:OD1	1.17	1.24
1:A:474:LEU:O	1:A:476:SER:O	1.67	1.13
1:B:473:ASP:O	1:B:476:SER:OG	1.66	1.13
1:B:473:ASP:HB3	1:B:477:MET:SD	1.89	1.13
1:D:534:ARG:HG3	1:D:534:ARG:HH11	1.03	1.10
1:A:410:THR:H	1:A:411:PRO:HD2	1.16	1.09
1:A:409:PHE:HA	1:A:412:ALA:HB3	1.13	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASP:O	1:B:477:MET:HG2	0.89	1.05
1:A:408:SER:O	1:A:411:PRO:HD2	1.59	1.03
1:C:463:PHE:HB2	1:C:467:LYS:HB2	1.05	1.01
1:A:402:TRP:O	1:A:406:SER:HB2	1.61	1.01
1:D:460:THR:HA	1:D:470:SER:HA	1.44	0.99
1:A:409:PHE:HA	1:A:412:ALA:CB	1.91	0.99
1:A:409:PHE:HD1	1:A:410:THR:N	1.60	0.98
1:B:473:ASP:C	1:B:477:MET:CG	2.25	0.97
1:A:470:SER:CB	1:A:473:ASP:OD1	2.13	0.95
1:B:404:GLU:HG2	1:B:467:LYS:HD2	1.48	0.95
1:B:473:ASP:CB	1:B:477:MET:SD	2.53	0.95
1:D:444:GLU:HG2	1:D:561:LEU:HB3	1.47	0.95
1:A:420:ALA:HA	1:A:423:ILE:HG13	1.49	0.93
1:A:398:GLY:HA2	1:A:477:MET:O	1.68	0.93
1:D:534:ARG:HH11	1:D:534:ARG:CG	1.81	0.93
1:B:471:VAL:HG12	1:B:474:LEU:HD12	1.50	0.92
1:A:410:THR:N	1:A:411:PRO:HD2	1.84	0.91
1:A:406:SER:OG	1:A:575:PHE:HE2	1.51	0.91
1:C:544:HIS:HB3	1:C:547:GLU:HB2	1.52	0.91
1:C:403:GLU:HA	1:C:406:SER:HB2	1.53	0.90
1:A:409:PHE:CD1	1:A:409:PHE:C	2.46	0.89
1:C:463:PHE:CB	1:C:467:LYS:HB2	1.99	0.89
1:D:413:VAL:HG13	1:D:442:THR:HG21	1.52	0.89
1:D:462:THR:HA	1:D:468:LYS:HA	1.55	0.88
1:B:516:ARG:HG3	1:B:516:ARG:HH11	1.37	0.87
1:A:409:PHE:HD1	1:A:409:PHE:C	1.78	0.86
1:B:474:LEU:O	1:B:477:MET:N	2.09	0.86
1:D:534:ARG:HG3	1:D:534:ARG:NH1	1.82	0.86
1:C:404:GLU:CG	1:C:467:LYS:HG3	2.08	0.84
1:B:471:VAL:HA	1:B:474:LEU:HG	1.60	0.83
1:A:406:SER:HB3	1:A:407:MET:HE3	1.60	0.82
1:C:463:PHE:HB2	1:C:467:LYS:CB	2.02	0.80
1:A:474:LEU:HD22	1:A:477:MET:CG	2.12	0.80
1:C:471:VAL:HG12	1:C:474:LEU:HD12	1.64	0.80
1:B:396:LYS:HD3	1:B:400:GLU:HG2	1.64	0.79
1:D:399:HIS:O	1:D:402:TRP:HB2	1.83	0.78
1:A:470:SER:HB3	1:A:473:ASP:CG	2.03	0.78
1:C:536:LEU:O	1:C:540:ILE:HG13	1.83	0.78
1:B:425:GLY:HA2	1:B:428:ASP:OD1	1.84	0.78
1:B:566:ASN:HB3	2:B:2024:HOH:O	1.83	0.78
1:B:401:ILE:HG13	1:B:469:TYR:CZ	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:O	1:D:421:LYS:HG2	1.85	0.77
1:A:403:GLU:O	1:A:407:MET:HG2	1.83	0.77
1:B:402:TRP:HE1	1:B:575:PHE:HZ	1.32	0.76
1:A:529:GLN:O	1:A:533:ILE:HB	1.86	0.76
1:A:474:LEU:HD22	1:A:477:MET:HG2	1.68	0.75
1:C:570:GLU:O	1:C:574:ALA:HB3	1.85	0.75
1:B:410:THR:HG21	1:B:576:LYS:HE2	1.68	0.75
1:C:402:TRP:HZ3	1:C:483:LEU:HD11	1.51	0.75
1:A:466:SER:HB2	1:C:431:GLN:HB2	1.69	0.75
1:D:449:ARG:HD2	2:D:2005:HOH:O	1.85	0.75
1:B:493:LEU:O	1:B:496:LEU:HB2	1.87	0.74
1:D:488:GLU:HB2	2:D:2014:HOH:O	1.88	0.74
1:A:397:SER:O	1:A:400:GLU:HB2	1.86	0.74
1:C:556:LEU:O	1:C:559:PRO:HD2	1.86	0.74
1:D:560:ASP:O	1:D:564:LEU:HG	1.87	0.73
1:A:516:ARG:O	1:A:519:ILE:HB	1.88	0.73
1:C:474:LEU:HD13	1:C:483:LEU:HB2	1.69	0.73
1:D:419:PHE:HA	1:D:422:ARG:HG3	1.69	0.73
1:A:544:HIS:HB3	1:A:547:GLU:HB2	1.70	0.73
1:C:404:GLU:CD	1:C:467:LYS:HG3	2.09	0.72
1:C:474:LEU:HD13	1:C:483:LEU:CB	2.19	0.72
1:C:425:GLY:HA2	1:C:428:ASP:OD1	1.89	0.72
1:C:553:LYS:O	1:C:557:LYS:HD3	1.89	0.72
1:B:515:ASP:OD1	1:B:517:SER:HB3	1.90	0.72
1:D:408:SER:O	1:D:411:PRO:HD2	1.91	0.71
1:C:402:TRP:HZ2	1:C:482:LEU:HD23	1.54	0.71
1:C:412:ALA:HA	1:C:415:GLU:OE2	1.90	0.71
1:C:540:ILE:HD11	1:C:554:LEU:HD12	1.73	0.71
1:B:398:GLY:HA3	1:B:477:MET:O	1.91	0.70
1:D:414:LYS:HD2	1:D:417:VAL:HG21	1.72	0.70
1:B:445:VAL:HG13	1:B:507:THR:HG23	1.73	0.70
1:D:482:LEU:HD22	1:D:568:HIS:HB3	1.73	0.70
1:A:481:ASP:O	1:A:484:ASN:HB3	1.90	0.70
1:A:563:SER:O	1:A:567:MET:HB2	1.92	0.70
1:C:402:TRP:CZ2	1:C:482:LEU:HD23	2.27	0.70
1:A:456:ALA:HB2	1:A:491:GLU:HB2	1.73	0.70
1:A:470:SER:O	1:A:473:ASP:OD2	2.09	0.70
1:B:447:MET:HG2	1:B:564:LEU:HD13	1.71	0.70
1:A:531:THR:O	1:A:534:ARG:HB2	1.92	0.69
1:B:396:LYS:N	1:B:400:GLU:HB3	2.06	0.69
1:C:462:THR:HG23	1:C:466:SER:HA	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ASN:O	1:C:525:VAL:HG23	1.93	0.69
1:C:474:LEU:HD22	1:C:483:LEU:CD1	2.23	0.69
1:C:430:SER:O	1:C:434:GLN:HG3	1.93	0.68
1:D:571:GLU:O	1:D:572:LEU:HD23	1.93	0.68
1:A:401:ILE:HG12	1:A:474:LEU:HD11	1.76	0.68
1:B:546:ASN:O	1:C:573:LEU:HD22	1.94	0.68
1:C:492:LYS:O	1:C:496:LEU:HD13	1.95	0.67
1:D:544:HIS:HB3	1:D:547:GLU:HB2	1.77	0.67
1:A:403:GLU:O	1:A:407:MET:CG	2.43	0.67
1:D:414:LYS:HE2	1:D:417:VAL:HG11	1.77	0.66
1:D:499:SER:OG	1:D:501:GLU:HB2	1.95	0.66
1:A:401:ILE:HG12	1:A:474:LEU:CD1	2.24	0.66
1:A:455:ASP:OD2	1:A:457:LYS:HD3	1.95	0.66
1:A:443:PHE:HE1	1:A:572:LEU:HD12	1.61	0.66
1:C:462:THR:OG1	1:C:468:LYS:HG3	1.96	0.66
1:B:403:GLU:HG2	1:B:407:MET:HE3	1.77	0.66
1:B:463:PHE:O	1:B:466:SER:N	2.29	0.66
1:B:536:LEU:O	1:B:540:ILE:HG13	1.95	0.66
1:B:455:ASP:OD2	1:B:457:LYS:HB2	1.96	0.66
1:B:530:GLU:O	1:B:534:ARG:HG3	1.96	0.66
1:A:521:ASN:HB3	1:A:524:SER:OG	1.96	0.66
1:A:408:SER:O	1:A:410:THR:N	2.25	0.65
1:A:463:PHE:O	1:A:466:SER:N	2.23	0.65
1:C:455:ASP:OD2	1:C:457:LYS:HB2	1.97	0.65
1:B:396:LYS:HD3	1:B:400:GLU:CG	2.26	0.65
1:C:471:VAL:HA	1:C:474:LEU:HB2	1.79	0.65
1:A:410:THR:N	1:A:411:PRO:CD	2.60	0.65
1:A:473:ASP:OD2	1:A:474:LEU:N	2.30	0.65
1:B:546:ASN:CA	1:B:547:GLU:OE2	2.45	0.65
1:B:546:ASN:C	1:B:547:GLU:OE2	2.34	0.65
1:D:453:LEU:HD11	1:D:464:LEU:CD1	2.27	0.65
1:B:451:ALA:HA	1:B:490:SER:HB2	1.79	0.65
1:B:471:VAL:HG12	1:B:474:LEU:CD1	2.27	0.64
1:B:545:PRO:HD2	1:C:439:LYS:HE3	1.79	0.64
1:A:536:LEU:O	1:A:540:ILE:HD12	1.97	0.64
1:C:437:LEU:HD13	1:C:519:ILE:HD11	1.79	0.64
1:C:474:LEU:HD23	1:C:477:MET:SD	2.37	0.64
1:C:482:LEU:HD21	1:C:572:LEU:HD21	1.79	0.64
1:A:409:PHE:CD1	1:A:410:THR:N	2.53	0.64
1:A:418:GLU:O	1:A:421:LYS:HB2	1.98	0.64
1:C:474:LEU:HA	1:C:477:MET:HB2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ARG:H	1:D:427:ARG:NE	1.95	0.64
1:D:423:ILE:HG22	1:D:426:PHE:HB2	1.80	0.63
1:D:516:ARG:HG2	1:D:522:VAL:HG13	1.79	0.63
1:C:432:HIS:CD2	1:C:520:GLU:HG3	2.33	0.63
1:C:463:PHE:O	1:C:466:SER:N	2.32	0.63
1:D:429:LEU:HB2	1:D:434:GLN:HG2	1.80	0.63
1:D:482:LEU:HD13	1:D:568:HIS:CD2	2.33	0.63
1:C:568:HIS:O	1:C:572:LEU:HG	1.98	0.63
1:D:471:VAL:HG11	1:D:487:PHE:CD1	2.34	0.63
1:B:404:GLU:HG3	1:B:463:PHE:HB2	1.79	0.62
1:B:505:LEU:HB3	1:B:536:LEU:HD13	1.81	0.62
1:A:559:PRO:HA	1:A:562:ARG:HB2	1.80	0.62
1:C:554:LEU:O	1:C:557:LYS:HG2	1.98	0.62
1:A:437:LEU:HD13	1:A:519:ILE:HD11	1.82	0.62
1:B:429:LEU:O	1:B:434:GLN:NE2	2.30	0.62
1:D:473:ASP:HB2	1:D:477:MET:SD	2.40	0.62
1:B:443:PHE:O	1:B:446:LEU:HB2	1.99	0.62
1:A:516:ARG:HA	1:A:519:ILE:HD13	1.80	0.62
1:A:526:GLU:HA	1:A:529:GLN:HG2	1.81	0.61
1:A:474:LEU:HA	1:A:477:MET:HB3	1.82	0.61
1:B:404:GLU:CG	1:B:467:LYS:HD2	2.28	0.61
1:C:414:LYS:HE2	1:C:418:GLU:OE1	1.99	0.61
1:B:455:ASP:HB2	2:B:2011:HOH:O	2.00	0.61
1:D:565:ASN:HD22	1:D:569:SER:HB3	1.65	0.61
1:C:516:ARG:HG2	1:C:522:VAL:HG13	1.83	0.61
1:B:471:VAL:HA	1:B:474:LEU:CG	2.28	0.61
1:B:403:GLU:O	1:B:406:SER:HB3	2.00	0.61
1:B:547:GLU:O	1:B:550:ILE:HG13	2.01	0.61
1:B:406:SER:HA	1:B:409:PHE:CE1	2.36	0.61
1:A:482:LEU:HD13	1:A:568:HIS:CD2	2.35	0.60
1:B:516:ARG:HG3	1:B:516:ARG:NH1	2.10	0.60
1:A:408:SER:O	1:A:411:PRO:CD	2.45	0.60
1:A:402:TRP:CZ2	1:A:572:LEU:HD21	2.36	0.60
1:D:568:HIS:HA	1:D:571:GLU:OE2	2.01	0.60
1:C:482:LEU:HD13	1:C:568:HIS:CD2	2.36	0.60
1:C:419:PHE:CE2	1:C:423:ILE:HD11	2.36	0.60
1:C:462:THR:CG2	1:C:466:SER:HA	2.31	0.60
1:B:458:GLU:HB3	1:B:460:THR:HG23	1.82	0.60
1:A:445:VAL:O	1:A:449:ARG:HB2	2.02	0.59
1:B:489:PHE:CE1	1:B:557:LYS:HD2	2.37	0.59
1:C:492:LYS:HE3	2:C:2013:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD22	1:B:479:ALA:HB3	1.84	0.59
1:B:408:SER:O	1:B:411:PRO:HD2	2.03	0.59
1:A:398:GLY:CA	1:A:477:MET:O	2.48	0.59
1:A:506:PHE:O	1:A:510:VAL:HG23	2.03	0.59
1:A:402:TRP:O	1:A:406:SER:CB	2.46	0.59
1:A:404:GLU:HA	1:A:404:GLU:OE1	2.00	0.58
1:A:407:MET:O	1:A:408:SER:HB2	2.02	0.58
1:C:474:LEU:HD22	1:C:483:LEU:HD12	1.85	0.58
1:A:566:ASN:HB3	2:A:2023:HOH:O	2.03	0.58
1:B:458:GLU:HB3	1:B:460:THR:CG2	2.33	0.58
1:B:482:LEU:O	1:B:486:MET:HG3	2.03	0.58
1:A:419:PHE:HA	1:A:422:ARG:NE	2.18	0.58
1:C:474:LEU:HD22	1:C:483:LEU:HD13	1.84	0.58
1:D:498:LEU:HD22	1:D:502:GLU:OE1	2.04	0.58
1:A:407:MET:O	1:A:408:SER:CB	2.51	0.58
1:B:397:SER:O	1:B:401:ILE:HD13	2.03	0.58
1:B:481:ASP:HA	1:B:484:ASN:HB3	1.84	0.58
1:B:473:ASP:HB2	1:B:477:MET:SD	2.39	0.58
1:B:536:LEU:HG	1:B:540:ILE:HD11	1.86	0.58
1:C:429:LEU:O	1:C:434:GLN:NE2	2.35	0.58
1:C:549:SER:O	1:C:553:LYS:HG3	2.03	0.58
1:B:403:GLU:O	1:B:407:MET:HG2	2.04	0.57
1:A:431:GLN:O	1:A:435:VAL:HG23	2.04	0.57
1:B:474:LEU:HA	1:B:477:MET:HB2	1.86	0.57
1:B:516:ARG:HA	1:B:519:ILE:HD13	1.84	0.57
1:A:409:PHE:CE2	1:A:572:LEU:HD22	2.39	0.57
1:D:534:ARG:CG	1:D:534:ARG:NH1	2.50	0.57
1:A:508:ALA:O	1:A:512:VAL:HG23	2.04	0.57
1:B:546:ASN:HB2	1:C:439:LYS:O	2.04	0.57
1:B:546:ASN:ND2	1:C:442:THR:HB	2.20	0.57
1:A:529:GLN:HG3	1:A:530:GLU:N	2.20	0.57
1:B:404:GLU:HG3	1:B:463:PHE:CB	2.34	0.57
1:C:484:ASN:O	1:C:488:GLU:HG2	2.05	0.57
1:B:474:LEU:N	1:B:477:MET:HG2	2.14	0.57
1:C:516:ARG:HG2	1:C:522:VAL:CG1	2.33	0.57
1:C:449:ARG:HB3	1:C:449:ARG:CZ	2.35	0.56
1:D:459:ARG:HB3	1:D:471:VAL:HG22	1.87	0.56
1:C:445:VAL:HG13	1:C:507:THR:HG23	1.87	0.56
1:C:461:VAL:HG12	1:C:469:TYR:HB2	1.88	0.56
1:D:420:ALA:HB1	1:D:426:PHE:CE2	2.40	0.56
1:A:406:SER:HB3	1:A:407:MET:CE	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:O	1:A:477:MET:HB3	2.05	0.56
1:D:505:LEU:O	1:D:509:VAL:HG23	2.05	0.56
1:C:534:ARG:O	1:C:538:THR:HG23	2.05	0.56
1:D:529:GLN:O	1:D:533:ILE:HD12	2.05	0.56
1:A:454:PHE:CD2	1:A:461:VAL:HB	2.41	0.56
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.71	0.56
1:B:489:PHE:CZ	1:B:561:LEU:HD21	2.40	0.56
1:D:483:LEU:HA	1:D:486:MET:HB2	1.88	0.56
1:C:526:GLU:O	1:C:530:GLU:HB2	2.06	0.56
1:D:431:GLN:O	1:D:435:VAL:HG23	2.06	0.56
1:D:456:ALA:HB2	1:D:491:GLU:HG3	1.88	0.56
1:A:429:LEU:O	1:A:434:GLN:NE2	2.33	0.55
1:D:456:ALA:CB	1:D:491:GLU:HG3	2.36	0.55
1:A:410:THR:HA	1:A:413:VAL:HG23	1.87	0.55
1:D:423:ILE:CG2	1:D:426:PHE:HB2	2.35	0.55
1:D:429:LEU:O	1:D:434:GLN:NE2	2.30	0.55
1:C:404:GLU:CG	1:C:467:LYS:CG	2.84	0.55
1:D:537:ARG:HG3	1:D:551:PHE:CZ	2.42	0.55
1:C:471:VAL:HA	1:C:474:LEU:CG	2.37	0.55
1:D:502:GLU:HA	1:D:539:LEU:HD21	1.88	0.55
1:D:409:PHE:O	1:D:413:VAL:HG23	2.06	0.55
1:D:406:SER:HA	1:D:409:PHE:CZ	2.41	0.55
1:D:484:ASN:O	1:D:488:GLU:HG2	2.06	0.55
1:A:443:PHE:CD2	1:A:565:ASN:HA	2.42	0.55
1:C:430:SER:OG	1:C:432:HIS:HB3	2.06	0.55
1:A:443:PHE:CE2	1:A:565:ASN:HA	2.41	0.55
1:B:506:PHE:O	1:B:509:VAL:HB	2.07	0.55
1:A:482:LEU:HD22	1:A:568:HIS:HB3	1.89	0.55
1:B:485:SER:HA	1:B:488:GLU:HG3	1.88	0.55
1:C:576:LYS:HG2	1:C:576:LYS:O	2.07	0.55
1:C:563:SER:O	1:C:567:MET:HB2	2.07	0.54
1:B:443:PHE:HE1	1:B:572:LEU:HG	1.71	0.54
1:D:509:VAL:HG22	1:D:532:LEU:HB3	1.88	0.54
1:D:556:LEU:O	1:D:559:PRO:HD2	2.06	0.54
1:C:467:LYS:HB3	1:C:469:TYR:HE2	1.72	0.54
1:D:403:GLU:O	1:D:407:MET:HG2	2.07	0.54
1:D:521:ASN:HB3	1:D:524:SER:OG	2.07	0.54
1:B:469:TYR:O	1:B:470:SER:CB	2.56	0.54
1:C:482:LEU:CD2	1:C:572:LEU:HD21	2.38	0.54
1:D:414:LYS:HE2	1:D:417:VAL:CG1	2.37	0.54
1:D:446:LEU:O	1:D:450:PHE:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:LEU:HD11	1:D:464:LEU:HD12	1.90	0.54
1:B:474:LEU:C	1:B:477:MET:H	2.10	0.54
1:D:405:PHE:O	1:D:408:SER:HB2	2.07	0.54
1:A:474:LEU:HA	1:A:477:MET:CB	2.37	0.53
1:C:403:GLU:CA	1:C:406:SER:HB2	2.34	0.53
1:D:444:GLU:HB3	1:D:561:LEU:HD13	1.88	0.53
1:B:401:ILE:CG2	1:B:401:ILE:O	2.56	0.53
1:B:473:ASP:O	1:B:477:MET:SD	2.66	0.53
1:D:419:PHE:CA	1:D:422:ARG:HG3	2.35	0.53
1:A:409:PHE:HE2	1:A:572:LEU:HD22	1.73	0.53
1:C:474:LEU:HD13	1:C:483:LEU:HB3	1.90	0.53
1:D:443:PHE:O	1:D:447:MET:HE3	2.09	0.53
1:A:544:HIS:HB3	1:A:547:GLU:CB	2.39	0.53
1:B:546:ASN:N	1:B:547:GLU:OE2	2.42	0.53
1:B:549:SER:OG	1:C:574:ALA:HB1	2.09	0.53
1:C:557:LYS:O	1:C:561:LEU:HD12	2.08	0.53
1:D:430:SER:O	1:D:434:GLN:HG3	2.09	0.53
1:A:492:LYS:O	1:A:496:LEU:HD13	2.09	0.53
1:B:516:ARG:HA	1:B:519:ILE:CD1	2.38	0.52
1:B:546:ASN:HD22	1:C:442:THR:HB	1.74	0.52
1:A:540:ILE:O	1:A:544:HIS:HB2	2.09	0.52
1:C:517:SER:HB3	2:C:2017:HOH:O	2.09	0.52
1:D:462:THR:OG1	1:D:468:LYS:HG2	2.10	0.52
1:B:546:ASN:CB	1:B:547:GLU:OE2	2.58	0.52
1:C:541:MET:HA	2:C:2019:HOH:O	2.09	0.52
1:B:537:ARG:CZ	1:B:541:MET:HE1	2.39	0.52
1:B:443:PHE:CE2	1:B:565:ASN:HA	2.44	0.52
1:B:471:VAL:O	1:B:474:LEU:HB2	2.09	0.52
1:B:419:PHE:HA	1:B:422:ARG:CZ	2.40	0.52
1:A:526:GLU:HG2	2:A:2015:HOH:O	2.10	0.52
1:C:432:HIS:CG	1:C:520:GLU:HG3	2.45	0.52
1:C:482:LEU:HD11	1:C:486:MET:HE2	1.92	0.52
1:A:401:ILE:HG13	1:A:469:TYR:CZ	2.44	0.51
1:D:473:ASP:O	1:D:477:MET:N	2.34	0.51
1:C:405:PHE:HB3	1:C:409:PHE:CZ	2.45	0.51
1:A:411:PRO:O	1:A:415:GLU:OE2	2.29	0.51
1:B:474:LEU:HA	1:B:477:MET:CG	2.40	0.51
1:B:516:ARG:NH1	1:B:516:ARG:CG	2.71	0.51
1:D:536:LEU:O	1:D:540:ILE:HG13	2.09	0.51
1:A:516:ARG:HA	1:A:519:ILE:CD1	2.39	0.51
1:B:451:ALA:HA	1:B:490:SER:CB	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:PHE:CE1	1:A:572:LEU:HD12	2.44	0.51
1:B:401:ILE:O	1:B:401:ILE:HG22	2.10	0.51
1:C:458:GLU:O	1:C:459:ARG:HB2	2.10	0.51
1:D:409:PHE:HB3	1:D:450:PHE:HE2	1.75	0.51
1:B:443:PHE:CD2	1:B:565:ASN:HA	2.46	0.51
1:C:469:TYR:O	1:C:470:SER:HB2	2.10	0.51
1:D:502:GLU:OE2	1:D:540:ILE:HA	2.11	0.51
1:A:482:LEU:HG	1:A:486:MET:HE3	1.93	0.51
1:C:444:GLU:HB2	1:C:510:VAL:HG11	1.92	0.51
1:B:403:GLU:HG2	1:B:407:MET:CE	2.39	0.51
1:B:404:GLU:HG2	1:B:467:LYS:CD	2.31	0.51
1:A:458:GLU:HB2	1:A:460:THR:HG23	1.93	0.50
1:C:453:LEU:HB3	1:C:462:THR:O	2.10	0.50
1:D:445:VAL:HG13	1:D:507:THR:HG23	1.93	0.50
1:D:476:SER:O	1:D:477:MET:C	2.49	0.50
1:A:406:SER:OG	1:A:575:PHE:CE2	2.39	0.50
1:B:411:PRO:O	1:B:415:GLU:OE2	2.28	0.50
1:B:558:LEU:HA	1:B:561:LEU:HD12	1.92	0.50
1:C:537:ARG:HG2	1:C:551:PHE:CZ	2.46	0.50
1:C:540:ILE:CD1	1:C:554:LEU:HD12	2.40	0.50
1:A:413:VAL:O	1:A:416:VAL:HB	2.12	0.50
1:B:432:HIS:O	1:B:436:ASN:OD1	2.30	0.50
1:B:512:VAL:HG12	1:B:529:GLN:HB3	1.94	0.50
1:D:515:ASP:OD1	1:D:517:SER:HB2	2.11	0.50
1:B:401:ILE:HG13	1:B:469:TYR:CE2	2.45	0.50
1:B:405:PHE:O	1:B:408:SER:HB2	2.11	0.50
1:D:432:HIS:CD2	1:D:520:GLU:HG3	2.46	0.50
1:A:556:LEU:O	1:A:559:PRO:HD2	2.11	0.50
1:B:411:PRO:HB2	2:B:2006:HOH:O	2.11	0.50
1:C:459:ARG:O	1:C:471:VAL:HG22	2.11	0.50
1:D:537:ARG:HG3	1:D:551:PHE:CE1	2.45	0.50
1:B:443:PHE:CE1	1:B:572:LEU:HG	2.46	0.50
1:C:484:ASN:O	1:C:487:PHE:HB3	2.11	0.50
1:D:509:VAL:CG2	1:D:532:LEU:HB3	2.42	0.50
1:A:406:SER:HG	1:A:575:PHE:HE2	0.69	0.50
1:C:471:VAL:HA	1:C:474:LEU:CB	2.42	0.50
1:C:519:ILE:HG21	1:C:525:VAL:HG21	1.93	0.50
1:D:419:PHE:CE2	1:D:507:THR:HG22	2.47	0.50
1:B:465:GLY:O	1:B:467:LYS:N	2.45	0.50
1:A:489:PHE:CZ	1:A:561:LEU:HD21	2.47	0.49
1:B:548:ALA:H	1:C:574:ALA:HB2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:CE2	1:A:434:GLN:HB3	2.47	0.49
1:D:494:ASN:HB2	2:D:2013:HOH:O	2.12	0.49
1:B:542:LYS:NZ	1:B:543:ASN:HD21	2.11	0.49
1:C:482:LEU:HD21	1:C:572:LEU:HD11	1.92	0.49
1:C:515:ASP:OD2	1:C:517:SER:HB2	2.11	0.49
1:C:567:MET:HG2	1:C:568:HIS:CD2	2.46	0.49
1:D:427:ARG:H	1:D:427:ARG:CD	2.25	0.49
1:A:396:LYS:N	1:A:400:GLU:HG2	2.27	0.49
1:B:505:LEU:O	1:B:509:VAL:HG23	2.11	0.49
1:C:505:LEU:HB3	1:C:536:LEU:HD13	1.95	0.49
1:D:459:ARG:HG2	1:D:487:PHE:CZ	2.47	0.49
1:A:406:SER:CB	1:A:407:MET:HE3	2.37	0.49
1:A:458:GLU:O	1:A:460:THR:HG22	2.13	0.49
1:B:414:LYS:HE2	1:B:418:GLU:HG2	1.95	0.49
1:C:474:LEU:CD2	1:C:483:LEU:HD13	2.42	0.49
1:C:560:ASP:O	1:C:564:LEU:HG	2.12	0.49
1:B:512:VAL:CG1	1:B:529:GLN:HB3	2.43	0.49
1:C:441:GLY:HA3	1:C:514:ALA:HB2	1.94	0.49
1:C:568:HIS:O	1:C:572:LEU:CD1	2.60	0.49
1:B:461:VAL:HG13	1:B:461:VAL:O	2.13	0.49
1:B:542:LYS:HZ2	1:B:543:ASN:HD21	1.60	0.49
1:D:398:GLY:HA3	1:D:477:MET:O	2.12	0.49
1:D:550:ILE:HD11	2:D:2015:HOH:O	2.12	0.49
1:A:408:SER:O	1:A:409:PHE:CD1	2.66	0.49
1:B:457:LYS:HD3	1:B:457:LYS:H	1.78	0.49
1:C:444:GLU:HB2	1:C:510:VAL:CG1	2.43	0.49
1:A:475:HIS:CD2	1:A:484:ASN:HB2	2.48	0.48
1:C:399:HIS:CD2	2:C:2008:HOH:O	2.65	0.48
1:D:512:VAL:HG11	1:D:528:LEU:HG	1.94	0.48
1:B:512:VAL:HG21	1:B:532:LEU:HD12	1.95	0.48
1:D:516:ARG:HA	1:D:519:ILE:HD12	1.96	0.48
1:A:443:PHE:CZ	1:A:447:MET:HE1	2.49	0.48
1:C:470:SER:O	1:C:474:LEU:HG	2.12	0.48
1:A:414:LYS:HD2	1:A:417:VAL:HB	1.95	0.48
1:B:417:VAL:O	1:B:421:LYS:HG3	2.12	0.48
1:B:465:GLY:O	1:B:467:LYS:HG3	2.14	0.48
1:A:412:ALA:O	1:A:415:GLU:HG2	2.13	0.48
1:A:512:VAL:HG11	1:A:528:LEU:HG	1.96	0.48
1:D:435:VAL:O	1:D:439:LYS:HB2	2.13	0.48
1:C:433:ASP:O	1:C:437:LEU:N	2.47	0.48
1:A:477:MET:O	1:A:477:MET:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:SER:H	1:C:574:ALA:CB	2.26	0.48
1:A:450:PHE:O	1:A:453:LEU:HB2	2.14	0.47
1:A:474:LEU:HD22	1:A:477:MET:CB	2.43	0.47
1:B:537:ARG:NH1	1:B:541:MET:HE1	2.29	0.47
1:D:499:SER:OG	1:D:501:GLU:CB	2.63	0.47
1:B:459:ARG:NH2	1:B:487:PHE:HE2	2.13	0.47
1:B:572:LEU:O	1:B:575:PHE:HD1	1.97	0.47
1:D:416:VAL:HA	1:D:419:PHE:HB3	1.95	0.47
1:A:432:HIS:HD2	1:A:433:ASP:OD1	1.98	0.47
1:D:503:MET:HG2	2:D:2016:HOH:O	2.14	0.47
1:A:396:LYS:N	1:A:400:GLU:HB3	2.29	0.47
1:A:433:ASP:O	1:A:437:LEU:HB2	2.15	0.47
1:A:528:LEU:O	1:A:532:LEU:HG	2.14	0.47
1:B:549:SER:CB	1:C:574:ALA:HB1	2.44	0.47
1:C:402:TRP:CZ3	1:C:483:LEU:HD21	2.50	0.47
1:D:437:LEU:CD1	1:D:519:ILE:HD11	2.45	0.47
1:D:463:PHE:HB2	1:D:467:LYS:HB2	1.97	0.47
1:D:420:ALA:CB	1:D:438:LEU:HD21	2.45	0.47
1:B:396:LYS:HB2	1:B:400:GLU:CB	2.45	0.47
1:B:474:LEU:N	1:B:477:MET:CG	2.75	0.47
1:D:538:THR:O	1:D:541:MET:HB2	2.15	0.47
1:C:484:ASN:ND2	1:C:488:GLU:OE2	2.48	0.47
1:D:526:GLU:O	1:D:530:GLU:OE1	2.32	0.47
1:D:499:SER:HG	1:D:501:GLU:HB2	1.79	0.46
1:C:444:GLU:HB3	1:C:561:LEU:HB3	1.97	0.46
1:C:471:VAL:HA	1:C:474:LEU:HG	1.97	0.46
1:D:431:GLN:OE1	1:D:435:VAL:HG23	2.15	0.46
1:D:443:PHE:HE1	1:D:572:LEU:HD12	1.80	0.46
1:D:455:ASP:OD2	1:D:457:LYS:HB2	2.14	0.46
1:A:410:THR:OG1	1:A:575:PHE:HB2	2.15	0.46
1:A:562:ARG:HE	1:A:562:ARG:HA	1.81	0.46
1:B:471:VAL:O	1:B:474:LEU:N	2.48	0.46
1:B:474:LEU:CA	1:B:477:MET:CG	2.93	0.46
1:C:420:ALA:O	1:C:423:ILE:HB	2.15	0.46
1:C:463:PHE:O	1:C:465:GLY:N	2.48	0.46
1:D:455:ASP:CG	1:D:458:GLU:HG2	2.36	0.46
1:D:498:LEU:HD12	1:D:503:MET:CE	2.45	0.46
1:A:474:LEU:CA	1:A:477:MET:HB3	2.45	0.46
1:A:551:PHE:O	1:A:554:LEU:HB2	2.16	0.46
1:D:512:VAL:HG12	1:D:512:VAL:O	2.16	0.46
1:B:545:PRO:HB2	1:C:440:ALA:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:LEU:HD13	1:C:568:HIS:CG	2.51	0.46
1:D:407:MET:HG2	1:D:407:MET:H	1.47	0.46
1:D:473:ASP:O	1:D:477:MET:HG3	2.16	0.46
1:B:546:ASN:O	1:B:547:GLU:HG3	2.16	0.46
1:C:429:LEU:HB2	1:C:434:GLN:CG	2.45	0.46
1:A:474:LEU:HD13	1:A:477:MET:HG2	1.96	0.46
1:C:420:ALA:HB1	1:C:426:PHE:CD2	2.51	0.46
1:C:458:GLU:OE1	1:C:458:GLU:HA	2.16	0.46
1:C:420:ALA:HB1	1:C:426:PHE:CE2	2.51	0.46
1:C:489:PHE:HE1	1:C:557:LYS:HB3	1.81	0.46
1:C:544:HIS:HB3	1:C:547:GLU:CB	2.36	0.46
1:D:414:LYS:HD2	1:D:417:VAL:CG2	2.43	0.46
1:A:405:PHE:HB2	1:A:463:PHE:CE1	2.51	0.45
1:B:414:LYS:HD2	1:B:414:LYS:HA	1.46	0.45
1:D:402:TRP:O	1:D:405:PHE:N	2.50	0.45
1:A:419:PHE:HA	1:A:422:ARG:CZ	2.46	0.45
1:A:489:PHE:O	1:A:557:LYS:NZ	2.50	0.45
1:D:400:GLU:C	1:D:401:ILE:HD12	2.36	0.45
1:A:456:ALA:CB	1:A:491:GLU:HB2	2.43	0.45
1:B:538:THR:HA	1:B:541:MET:HB2	1.98	0.45
1:B:506:PHE:O	1:B:510:VAL:N	2.50	0.45
1:C:473:ASP:O	1:C:477:MET:N	2.50	0.45
1:C:478:GLY:O	1:C:480:GLY:N	2.50	0.45
1:C:516:ARG:HA	1:C:519:ILE:CD1	2.46	0.45
1:D:419:PHE:O	1:D:422:ARG:HG3	2.15	0.45
1:D:427:ARG:NH2	1:D:428:ASP:OD1	2.50	0.45
1:D:534:ARG:O	1:D:538:THR:HG23	2.16	0.45
1:A:550:ILE:O	1:A:554:LEU:HG	2.17	0.45
1:B:481:ASP:OD2	1:B:481:ASP:N	2.50	0.45
1:B:506:PHE:O	1:B:509:VAL:N	2.50	0.45
1:B:544:HIS:N	1:B:545:PRO:HD3	2.31	0.45
1:C:484:ASN:HB2	2:C:2011:HOH:O	2.17	0.45
1:A:455:ASP:O	1:A:459:ARG:N	2.50	0.45
1:B:557:LYS:O	1:B:561:LEU:HG	2.16	0.45
1:C:412:ALA:O	1:C:415:GLU:HG2	2.16	0.45
1:C:474:LEU:CA	1:C:477:MET:HB2	2.47	0.45
1:D:445:VAL:HG21	1:D:511:LEU:HB2	1.98	0.45
1:D:474:LEU:O	1:D:475:HIS:C	2.54	0.45
1:D:492:LYS:NZ	2:D:2014:HOH:O	2.50	0.45
1:D:561:LEU:O	1:D:564:LEU:HB2	2.17	0.45
1:B:432:HIS:CD2	1:B:520:GLU:HG3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:PHE:O	1:B:446:LEU:N	2.50	0.45
1:B:489:PHE:O	1:B:557:LYS:NZ	2.50	0.45
1:B:509:VAL:O	1:B:513:SER:OG	2.30	0.45
1:B:529:GLN:HG3	1:B:530:GLU:N	2.31	0.45
1:C:568:HIS:O	1:C:572:LEU:CG	2.64	0.45
1:B:409:PHE:O	1:B:412:ALA:HB3	2.16	0.45
1:D:424:PRO:HA	2:D:2003:HOH:O	2.17	0.45
1:C:482:LEU:O	1:C:486:MET:HG3	2.17	0.44
1:A:402:TRP:HZ3	1:A:483:LEU:HG	1.82	0.44
1:A:446:LEU:O	1:A:450:PHE:N	2.50	0.44
1:B:482:LEU:HG	1:B:486:MET:CE	2.48	0.44
1:C:405:PHE:HB3	1:C:409:PHE:HZ	1.81	0.44
1:D:421:LYS:HG2	1:D:421:LYS:HZ3	1.69	0.44
1:D:423:ILE:CD1	1:D:511:LEU:HD23	2.47	0.44
1:A:573:LEU:O	1:A:575:PHE:N	2.49	0.44
1:B:414:LYS:NZ	1:B:418:GLU:OE1	2.48	0.44
1:B:474:LEU:HA	1:B:474:LEU:HD23	1.85	0.44
1:B:502:GLU:OE2	1:B:544:HIS:NE2	2.50	0.44
1:B:529:GLN:O	1:B:533:ILE:HB	2.17	0.44
1:C:437:LEU:HD12	1:C:514:ALA:HB3	1.98	0.44
1:C:502:GLU:HG2	1:C:539:LEU:HG	1.98	0.44
1:D:413:VAL:HG13	1:D:442:THR:CG2	2.35	0.44
1:D:451:ALA:HB1	1:D:490:SER:HA	2.00	0.44
1:B:474:LEU:CA	1:B:477:MET:HG2	2.47	0.44
1:B:549:SER:H	1:C:574:ALA:HB1	1.83	0.44
1:C:429:LEU:HB2	1:C:434:GLN:HG2	1.99	0.44
1:D:490:SER:O	1:D:494:ASN:OD1	2.34	0.44
1:D:522:VAL:HG12	1:D:526:GLU:OE2	2.17	0.44
1:D:565:ASN:ND2	2:D:2025:HOH:O	2.50	0.44
1:A:418:GLU:HA	1:A:421:LYS:HG3	1.99	0.44
1:A:566:ASN:ND2	2:A:2022:HOH:O	2.50	0.44
1:B:489:PHE:HE1	1:B:557:LYS:HD2	1.81	0.44
1:B:499:SER:O	1:B:502:GLU:N	2.50	0.44
1:C:417:VAL:HG12	1:C:418:GLU:OE1	2.17	0.44
1:D:409:PHE:HB3	1:D:450:PHE:CE2	2.53	0.44
1:A:443:PHE:O	1:A:447:MET:HE2	2.17	0.44
1:C:463:PHE:O	1:C:464:LEU:C	2.55	0.44
1:D:460:THR:HG22	1:D:470:SER:HB2	1.98	0.44
1:B:502:GLU:CD	1:B:544:HIS:HE2	2.21	0.44
1:C:405:PHE:O	1:C:409:PHE:CE1	2.71	0.44
1:C:421:LYS:H	1:C:421:LYS:HG2	1.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:ASP:OD1	1:D:428:ASP:N	2.50	0.44
1:B:408:SER:O	1:B:412:ALA:HB2	2.18	0.44
1:C:496:LEU:HD23	1:C:554:LEU:HD23	2.00	0.44
1:D:455:ASP:OD2	1:D:458:GLU:N	2.50	0.44
1:A:408:SER:C	1:A:411:PRO:HD2	2.35	0.44
1:B:420:ALA:HA	1:B:423:ILE:HD12	2.00	0.44
1:D:467:LYS:O	1:D:469:TYR:HD2	2.01	0.44
1:D:482:LEU:HD22	1:D:568:HIS:CB	2.46	0.44
1:B:412:ALA:O	1:B:415:GLU:HG2	2.18	0.43
1:C:414:LYS:HD2	1:C:414:LYS:O	2.18	0.43
1:D:414:LYS:NZ	1:D:418:GLU:OE1	2.50	0.43
1:D:455:ASP:OD2	1:D:457:LYS:N	2.50	0.43
1:D:469:TYR:HB3	1:D:470:SER:H	1.55	0.43
1:D:537:ARG:HG3	1:D:551:PHE:CE2	2.53	0.43
1:D:427:ARG:H	1:D:427:ARG:HE	1.62	0.43
1:D:482:LEU:HG	1:D:486:MET:CE	2.48	0.43
1:B:456:ALA:HB1	1:B:491:GLU:OE2	2.19	0.43
1:C:546:ASN:N	1:C:547:GLU:OE2	2.50	0.43
1:D:413:VAL:HG22	1:D:446:LEU:HD11	1.99	0.43
1:D:458:GLU:HB2	1:D:460:THR:OG1	2.18	0.43
1:D:572:LEU:O	1:D:575:PHE:CD1	2.71	0.43
1:C:512:VAL:HG12	1:C:512:VAL:O	2.18	0.43
1:D:399:HIS:HB2	1:D:478:GLY:O	2.18	0.43
1:D:414:LYS:HE2	1:D:417:VAL:CB	2.49	0.43
1:A:482:LEU:HD21	1:A:572:LEU:HD11	2.01	0.43
1:B:540:ILE:HG23	1:B:544:HIS:CD2	2.54	0.43
1:C:510:VAL:HG21	1:C:561:LEU:HD13	2.00	0.43
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.74	0.43
1:A:433:ASP:O	1:A:437:LEU:N	2.50	0.43
1:B:414:LYS:CE	1:B:418:GLU:OE1	2.67	0.43
1:C:443:PHE:CE2	1:C:565:ASN:HA	2.54	0.43
1:C:516:ARG:HA	1:C:519:ILE:HD13	1.99	0.43
1:A:543:ASN:C	1:A:545:PRO:HD3	2.39	0.43
1:D:414:LYS:HA	1:D:417:VAL:HG23	2.01	0.43
1:A:443:PHE:CE1	1:A:447:MET:HE1	2.53	0.43
1:B:414:LYS:HE3	1:B:417:VAL:HB	1.99	0.43
1:B:433:ASP:O	1:B:437:LEU:HD22	2.19	0.43
1:A:455:ASP:OD2	1:A:458:GLU:N	2.50	0.43
1:A:557:LYS:O	1:A:560:ASP:HB2	2.19	0.43
1:B:410:THR:HG21	1:B:576:LYS:CE	2.43	0.43
1:B:410:THR:HG22	1:B:411:PRO:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:GLU:HG2	1:C:415:GLU:H	1.53	0.43
1:D:484:ASN:HB2	2:D:2012:HOH:O	2.17	0.43
1:D:576:LYS:HB3	1:D:576:LYS:HE3	1.55	0.43
1:A:401:ILE:HG13	1:A:469:TYR:CE1	2.53	0.43
1:A:475:HIS:NE2	1:A:481:ASP:OD2	2.52	0.43
1:A:484:ASN:O	1:A:487:PHE:N	2.50	0.43
1:A:562:ARG:HA	1:A:562:ARG:NE	2.34	0.43
1:B:402:TRP:NE1	1:B:575:PHE:HZ	2.07	0.43
1:D:549:SER:O	1:D:552:THR:N	2.52	0.43
1:A:405:PHE:CE1	1:A:409:PHE:HD2	2.37	0.42
1:A:455:ASP:CG	1:A:457:LYS:HD3	2.38	0.42
1:B:409:PHE:O	1:B:413:VAL:HG23	2.19	0.42
1:B:482:LEU:HG	1:B:486:MET:HE3	2.01	0.42
1:C:568:HIS:O	1:C:572:LEU:HD12	2.19	0.42
1:D:437:LEU:HD21	1:D:512:VAL:HA	2.01	0.42
1:D:443:PHE:CE2	1:D:565:ASN:HA	2.54	0.42
1:D:564:LEU:N	1:D:564:LEU:HD23	2.34	0.42
1:A:401:ILE:HG12	1:A:474:LEU:HD13	1.98	0.42
1:C:399:HIS:HD2	2:C:2008:HOH:O	1.99	0.42
1:D:547:GLU:O	1:D:550:ILE:HG13	2.19	0.42
1:B:474:LEU:HD22	1:B:479:ALA:CB	2.49	0.42
1:D:453:LEU:HD11	1:D:464:LEU:HD11	2.00	0.42
1:D:474:LEU:N	1:D:474:LEU:HD23	2.34	0.42
1:D:537:ARG:HE	1:D:537:ARG:HB3	1.64	0.42
1:A:574:ALA:O	1:A:575:PHE:HD1	2.03	0.42
1:C:558:LEU:HB2	1:C:559:PRO:HD3	2.01	0.42
1:D:433:ASP:O	1:D:437:LEU:HB2	2.19	0.42
1:D:530:GLU:O	1:D:534:ARG:HB2	2.20	0.42
1:A:460:THR:O	1:A:460:THR:OG1	2.30	0.42
1:C:543:ASN:C	1:C:545:PRO:HD3	2.40	0.42
1:C:446:LEU:O	1:C:450:PHE:CD1	2.72	0.42
1:B:403:GLU:OE2	1:B:407:MET:HE1	2.20	0.42
1:B:543:ASN:C	1:B:545:PRO:HD3	2.40	0.42
1:C:459:ARG:NH1	1:C:459:ARG:HG2	2.35	0.41
1:C:576:LYS:HB3	1:C:576:LYS:HE2	1.82	0.41
1:B:445:VAL:HG13	1:B:507:THR:CG2	2.43	0.41
1:C:404:GLU:OE1	1:C:467:LYS:HG3	2.19	0.41
1:D:406:SER:HA	1:D:409:PHE:CE1	2.54	0.41
1:D:467:LYS:O	1:D:469:TYR:CD2	2.73	0.41
1:A:559:PRO:O	1:A:562:ARG:HB3	2.21	0.41
1:B:447:MET:CG	1:B:564:LEU:HD13	2.47	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:HIS:HE1	2:B:2003:HOH:O	2.03	0.41
1:B:421:LYS:NZ	1:D:472:ASP:OD1	2.47	0.41
1:C:465:GLY:O	1:C:466:SER:C	2.58	0.41
1:C:475:HIS:CD2	2:C:2011:HOH:O	2.73	0.41
1:C:402:TRP:O	1:C:405:PHE:HB2	2.21	0.41
1:D:438:LEU:O	1:D:442:THR:OG1	2.30	0.41
1:A:543:ASN:O	1:A:545:PRO:HD3	2.21	0.41
1:B:417:VAL:HG12	1:B:421:LYS:NZ	2.36	0.41
1:B:421:LYS:HD3	1:D:472:ASP:HB3	2.02	0.41
1:C:547:GLU:HB3	1:C:550:ILE:HG13	2.02	0.41
1:D:500:ASP:OD1	1:D:500:ASP:N	2.52	0.41
1:B:515:ASP:HB3	2:B:2017:HOH:O	2.19	0.41
1:C:409:PHE:CE2	1:C:572:LEU:HD22	2.56	0.41
1:D:410:THR:HG22	1:D:411:PRO:N	2.35	0.41
1:D:423:ILE:HA	1:D:424:PRO:HD3	1.72	0.41
1:A:455:ASP:OD2	1:A:458:GLU:HG2	2.20	0.41
1:B:402:TRP:O	1:B:406:SER:HB2	2.20	0.41
1:B:507:THR:O	1:B:510:VAL:HB	2.21	0.41
1:B:521:ASN:O	1:B:524:SER:OG	2.33	0.41
1:B:557:LYS:HD3	1:B:557:LYS:HA	1.90	0.41
1:C:455:ASP:O	1:C:459:ARG:N	2.50	0.41
1:C:459:ARG:HG2	1:C:459:ARG:HH11	1.86	0.41
1:D:405:PHE:CD2	1:D:409:PHE:HE2	2.37	0.41
1:D:505:LEU:HD23	1:D:505:LEU:HA	1.75	0.41
1:D:514:ALA:HB2	2:D:2004:HOH:O	2.20	0.41
1:D:537:ARG:HA	1:D:551:PHE:CD2	2.55	0.41
1:D:418:GLU:O	1:D:421:LYS:HB2	2.21	0.41
1:D:437:LEU:HD12	1:D:519:ILE:HD11	2.03	0.41
1:D:455:ASP:OD1	1:D:458:GLU:HG2	2.21	0.41
1:D:461:VAL:O	1:D:469:TYR:N	2.54	0.41
1:A:405:PHE:CZ	1:A:409:PHE:HD2	2.39	0.40
1:A:572:LEU:HA	1:A:572:LEU:HD23	1.85	0.40
1:B:570:GLU:O	1:B:574:ALA:HB3	2.21	0.40
1:C:404:GLU:HG2	1:C:467:LYS:CG	2.51	0.40
1:C:555:LEU:O	1:C:558:LEU:HG	2.21	0.40
1:D:502:GLU:CA	1:D:539:LEU:HD21	2.51	0.40
1:B:546:ASN:HB3	1:C:573:LEU:HD22	2.03	0.40
1:C:449:ARG:NH1	1:C:450:PHE:HE1	2.19	0.40
1:D:413:VAL:CG2	1:D:446:LEU:HD11	2.52	0.40
1:D:572:LEU:O	1:D:575:PHE:HD1	2.04	0.40
1:B:474:LEU:HA	1:B:477:MET:CB	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ASP:O	1:C:477:MET:HB2	2.21	0.40
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.98	0.40
1:C:443:PHE:CD2	1:C:565:ASN:HA	2.55	0.40
1:D:414:LYS:HE2	1:D:417:VAL:HB	2.04	0.40
1:D:516:ARG:NH1	1:D:516:ARG:HG3	2.36	0.40
1:A:474:LEU:HD22	1:A:477:MET:SD	2.60	0.40
1:C:423:ILE:HA	1:C:424:PRO:HD3	1.85	0.40
1:C:430:SER:HG	1:C:432:HIS:HB3	1.86	0.40
1:D:488:GLU:O	1:D:492:LYS:HG3	2.22	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	179/194 (92%)	146 (82%)	28 (16%)	5 (3%)	5 4
1	B	179/194 (92%)	154 (86%)	21 (12%)	4 (2%)	6 7
1	C	177/194 (91%)	142 (80%)	26 (15%)	9 (5%)	2 1
1	D	177/194 (91%)	146 (82%)	29 (16%)	2 (1%)	14 20
All	All	712/776 (92%)	588 (83%)	104 (15%)	20 (3%)	5 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLY
1	A	408	SER
1	A	409	PHE
1	B	470	SER
1	A	470	SER
1	A	480	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	464	LEU
1	C	470	SER
1	C	480	GLY
1	C	400	GLU
1	B	466	SER
1	C	432	HIS
1	C	434	GLN
1	D	477	MET
1	C	479	ALA
1	C	574	ALA
1	D	457	LYS
1	B	467	LYS
1	B	547	GLU
1	C	545	PRO

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	161/174 (92%)	115 (71%)	46 (29%)	0 0
1	B	161/174 (92%)	119 (74%)	42 (26%)	0 0
1	C	159/174 (91%)	120 (76%)	39 (24%)	0 0
1	D	159/174 (91%)	114 (72%)	45 (28%)	0 0
All	All	640/696 (92%)	468 (73%)	172 (27%)	0 0

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	LYS
1	A	397	SER
1	A	399	HIS
1	A	400	GLU
1	A	402	TRP
1	A	404	GLU
1	A	407	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	409	PHE
1	A	414	LYS
1	A	415	GLU
1	A	422	ARG
1	A	427	ARG
1	A	430	SER
1	A	435	VAL
1	A	447	MET
1	A	449	ARG
1	A	457	LYS
1	A	460	THR
1	A	464	LEU
1	A	466	SER
1	A	468	LYS
1	A	474	LEU
1	A	475	HIS
1	A	481	ASP
1	A	482	LEU
1	A	485	SER
1	A	488	GLU
1	A	491	GLU
1	A	497	GLN
1	A	500	ASP
1	A	504	SER
1	A	505	LEU
1	A	519	ILE
1	A	520	GLU
1	A	525	VAL
1	A	533	ILE
1	A	537	ARG
1	A	538	THR
1	A	552	THR
1	A	563	SER
1	A	565	ASN
1	A	567	MET
1	A	569	SER
1	A	571	GLU
1	A	573	LEU
1	A	576	LYS
1	B	396	LYS
1	B	397	SER
1	B	404	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	407	MET
1	B	409	PHE
1	B	410	THR
1	B	414	LYS
1	B	427	ARG
1	B	435	VAL
1	B	437	LEU
1	B	447	MET
1	B	449	ARG
1	B	457	LYS
1	B	458	GLU
1	B	459	ARG
1	B	468	LYS
1	B	472	ASP
1	B	481	ASP
1	B	488	GLU
1	B	492	LYS
1	B	499	SER
1	B	500	ASP
1	B	504	SER
1	B	505	LEU
1	B	510	VAL
1	B	513	SER
1	B	515	ASP
1	B	516	ARG
1	B	517	SER
1	B	519	ILE
1	B	526	GLU
1	B	531	THR
1	B	533	ILE
1	B	534	ARG
1	B	537	ARG
1	B	538	THR
1	B	562	ARG
1	B	565	ASN
1	B	567	MET
1	B	570	GLU
1	B	572	LEU
1	B	573	LEU
1	C	400	GLU
1	C	402	TRP
1	C	403	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	404	GLU
1	C	405	PHE
1	C	406	SER
1	C	407	MET
1	C	409	PHE
1	C	410	THR
1	C	414	LYS
1	C	415	GLU
1	C	421	LYS
1	C	427	ARG
1	C	428	ASP
1	C	430	SER
1	C	437	LEU
1	C	449	ARG
1	C	457	LYS
1	C	468	LYS
1	C	477	MET
1	C	485	SER
1	C	488	GLU
1	C	492	LYS
1	C	497	GLN
1	C	499	SER
1	C	504	SER
1	C	505	LEU
1	C	519	ILE
1	C	524	SER
1	C	526	GLU
1	C	533	ILE
1	C	534	ARG
1	C	537	ARG
1	C	541	MET
1	C	550	ILE
1	C	554	LEU
1	C	557	LYS
1	C	565	ASN
1	C	573	LEU
1	D	399	HIS
1	D	400	GLU
1	D	403	GLU
1	D	404	GLU
1	D	407	MET
1	D	410	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	414	LYS
1	D	421	LYS
1	D	422	ARG
1	D	427	ARG
1	D	428	ASP
1	D	431	GLN
1	D	439	LYS
1	D	446	LEU
1	D	447	MET
1	D	449	ARG
1	D	453	LEU
1	D	470	SER
1	D	473	ASP
1	D	474	LEU
1	D	476	SER
1	D	484	ASN
1	D	485	SER
1	D	488	GLU
1	D	497	GLN
1	D	498	LEU
1	D	499	SER
1	D	500	ASP
1	D	501	GLU
1	D	504	SER
1	D	505	LEU
1	D	516	ARG
1	D	529	GLN
1	D	531	THR
1	D	533	ILE
1	D	534	ARG
1	D	537	ARG
1	D	542	LYS
1	D	547	GLU
1	D	549	SER
1	D	562	ARG
1	D	565	ASN
1	D	567	MET
1	D	571	GLU
1	D	576	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	565	ASN
1	A	566	ASN
1	A	568	HIS
1	B	436	ASN
1	B	543	ASN
1	B	546	ASN
1	B	565	ASN
1	C	399	HIS
1	C	431	GLN
1	C	432	HIS
1	C	484	ASN
1	C	565	ASN
1	D	432	HIS
1	D	484	ASN
1	D	565	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	181/194 (93%)	-1.04	1 (0%)	89	88	9, 28, 89, 135	0
1	B	181/194 (93%)	-1.00	2 (1%)	80	79	8, 30, 97, 129	0
1	C	179/194 (92%)	-0.98	2 (1%)	80	79	5, 29, 81, 122	0
1	D	179/194 (92%)	-0.90	4 (2%)	62	60	7, 35, 115, 138	0
All	All	720/776 (92%)	-0.98	9 (1%)	77	75	5, 31, 94, 138	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	474	LEU	11.7
1	D	475	HIS	4.0
1	D	474	LEU	3.3
1	C	475	HIS	3.1
1	D	575	PHE	2.8
1	B	575	PHE	2.8
1	B	574	ALA	2.6
1	A	475	HIS	2.5
1	D	573	LEU	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.