Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 09:56 pm GMT

PDB ID	:	1HCI
Title	:	CRYSTAL STRUCTURE OF THE ROD DOMAIN OF ALPHA-ACTININ
Authors	:	Ylanne, J.; Scheffzek, K.; Young, P.; Saraste, M.
Deposited on	:	2001-05-04
Resolution	:	2.80 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:

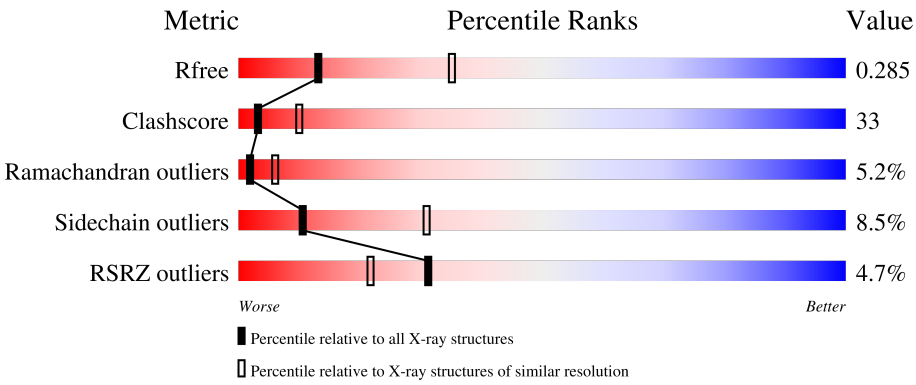
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	476	5% 48% 43% 8%
1	B	476	4% 48% 42% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7900 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 ALPHA-ACTININ 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	475	3942	2453	714	758	17	0	0	0
1	B	475	3942	2453	714	758	17	0	0	0

- Molecule 2 is water.

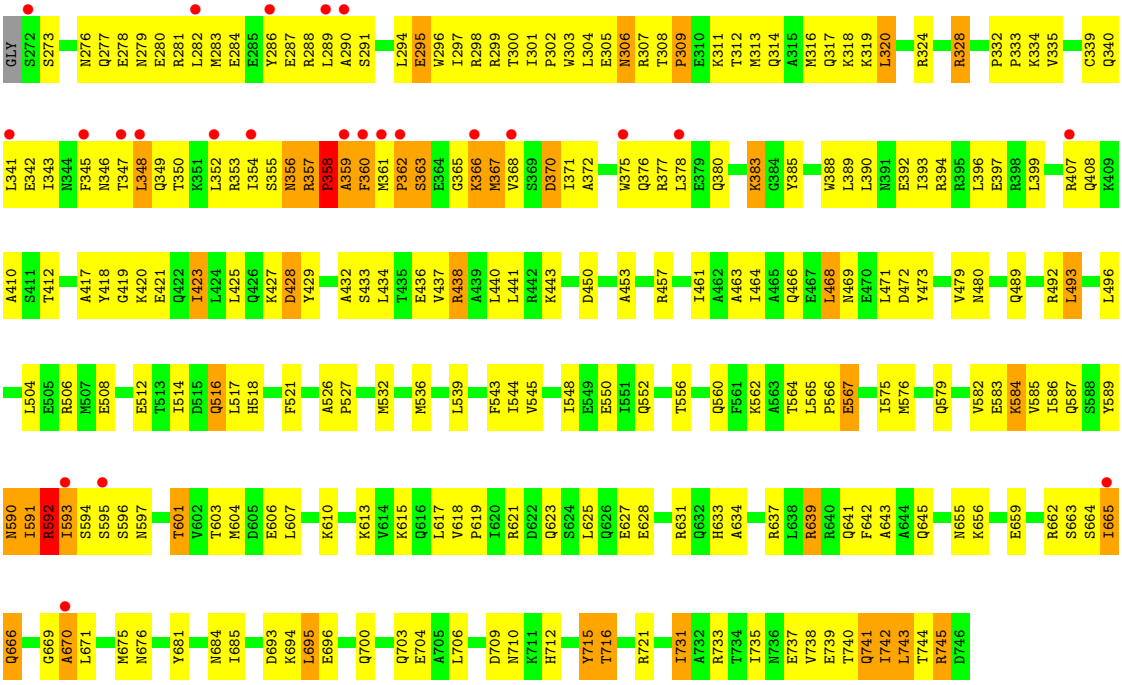
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	7	7	7	0	0
2	B	9	9	9	0	0

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.

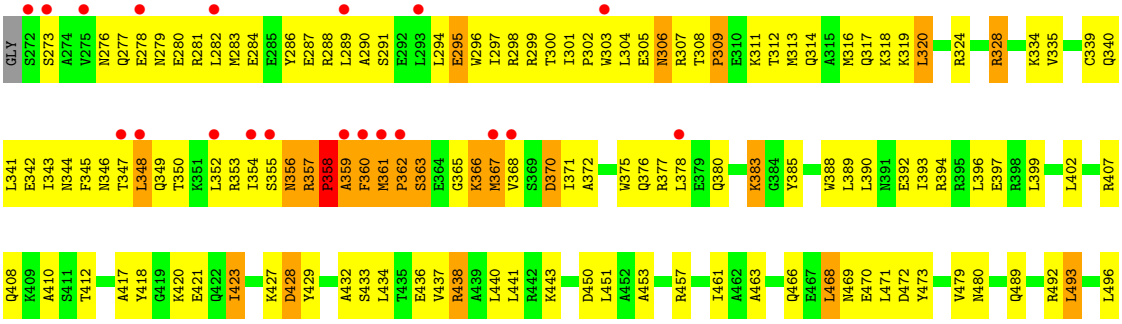
• Molecule 1: ALPHA-ACTININ 2

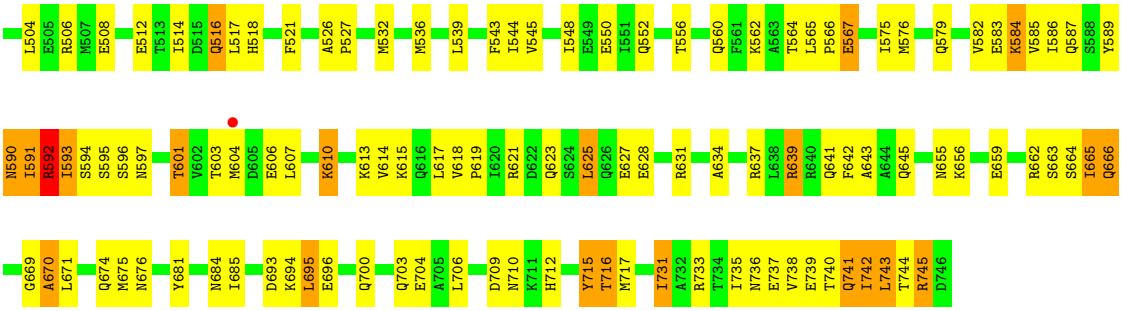
Chain A:



• Molecule 1: ALPHA-ACTININ 2

Chain B:




L504 E505 R506 M507 E508 E512 T513 I514 D515 Q516 L517 H518 F521 A526 P527 M532 M536 L539 F543 I544 V545 I548 E549 E550 I551 Q552 T556 Q560 F561 K562 A563 T564 L565 P566 E567 I575 M576 Q579 V582 E583 K584 V585 I586 Q587 S588 Y589
N590 I591 R592 I593 S594 S595 S596 N597 T601 V602 T603 M604 D605 E606 L607 K610 K613 V614 K615 Q616 L617 V618 P619 I620 R621 D622 Q623 S624 L625 Q626 E627 E628 R631 A634 R637 L638 R639 R640 Q641 F642 A643 A644 Q645 N655 K656 E659 R662 S663 S664 I665 Q666
G669 A670 L671 Q674 M675 N676 Y681 N684 I685 D693 K694 L695 E696 Q700 Q703 E704 A705 L706 D709 N710 K711 H712 Y715 T716 M717 I731 A732 R733 T734 I735 N736 E737 V738 E739 T740 Q741 I742 L743 T744 R745 D746

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	103.28Å 103.28Å 218.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.78 – 2.80 82.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (82.78-2.80) 98.7 (82.78-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.69Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.270 , 0.295 0.261 , 0.285	Depositor DCC
R_{free} test set	7073 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.450 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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	0.41	0/4008	0.63	1/5401 (0.0%)
1	B	0.42	0/4008	0.63	1/5401 (0.0%)
All	All	0.42	0/8016	0.63	2/10802 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	715	TYR	N-CA-C	5.05	124.63	111.00
1	A	715	TYR	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3942	0	3889	268	0
1	B	3942	0	3889	273	0
2	A	7	0	0	0	0
2	B	9	0	0	0	0
All	All	7900	0	7778	523	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 33.

All (523) 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:A:526:ALA:HB3	1:A:527:PRO:HD3	1.41	1.02
1:B:526:ALA:HB3	1:B:527:PRO:HD3	1.39	1.02
1:B:469:ASN:HD21	1:B:480:ASN:HD21	1.15	0.95
1:A:469:ASN:HD21	1:A:480:ASN:HD21	1.17	0.92
1:B:665:ILE:CD1	1:B:666:GLN:H	1.83	0.91
1:A:350:THR:HG23	1:A:353:ARG:HH12	1.35	0.91
1:A:665:ILE:CD1	1:A:666:GLN:H	1.82	0.91
1:B:350:THR:HG23	1:B:353:ARG:HH12	1.36	0.90
1:B:342:GLU:HA	1:B:345:PHE:HB3	1.54	0.88
1:A:342:GLU:HA	1:A:345:PHE:HB3	1.54	0.87
1:A:665:ILE:HD13	1:A:666:GLN:H	1.41	0.84
1:B:665:ILE:HD13	1:B:666:GLN:H	1.42	0.83
1:A:576:MET:HG2	1:A:604:MET:SD	2.19	0.83
1:A:740:THR:HG23	1:B:350:THR:HG21	1.61	0.82
1:B:576:MET:HG2	1:B:604:MET:SD	2.20	0.81
1:A:350:THR:HG21	1:B:740:THR:HG23	1.62	0.81
1:B:367:MET:HB2	1:B:370:ASP:HB2	1.63	0.79
1:A:350:THR:HG23	1:A:353:ARG:NH1	1.98	0.78
1:A:367:MET:HB2	1:A:370:ASP:HB2	1.63	0.78
1:B:576:MET:HA	1:B:604:MET:HE1	1.66	0.76
1:B:350:THR:HG23	1:B:353:ARG:NH1	1.99	0.76
1:B:700:GLN:O	1:B:704:GLU:HG3	1.85	0.76
1:B:357:ARG:O	1:B:357:ARG:HG3	1.85	0.75
1:B:279:ASN:HD21	1:B:352:LEU:HD21	1.51	0.75
1:A:357:ARG:O	1:A:357:ARG:HG3	1.85	0.75
1:A:279:ASN:HD21	1:A:352:LEU:HD21	1.51	0.75
1:B:349:GLN:HE22	1:B:359:ALA:HB1	1.51	0.74
1:A:349:GLN:HE22	1:A:359:ALA:HB1	1.51	0.74
1:B:603:THR:HG23	1:B:606:GLU:H	1.53	0.73
1:A:278:GLU:HA	1:A:281:ARG:HG2	1.72	0.72
1:A:603:THR:HG23	1:A:606:GLU:H	1.54	0.72
1:B:273:SER:HA	1:B:276:ASN:HD22	1.52	0.72
1:A:273:SER:HA	1:A:276:ASN:HD22	1.52	0.72
1:A:681:TYR:O	1:A:685:ILE:HG12	1.89	0.71
1:A:576:MET:HA	1:A:604:MET:HE1	1.72	0.71
1:B:681:TYR:O	1:B:685:ILE:HG12	1.91	0.71
1:B:278:GLU:HA	1:B:281:ARG:HG2	1.71	0.71
1:A:694:LYS:HB2	1:A:694:LYS:NZ	2.06	0.71
1:B:671:LEU:HD23	1:B:671:LEU:H	1.56	0.70
1:B:694:LYS:HB2	1:B:694:LYS:NZ	2.05	0.70
1:A:671:LEU:H	1:A:671:LEU:HD23	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ILE:CD1	1:A:666:GLN:N	2.54	0.70
1:A:589:TYR:HB2	1:A:591:ILE:HG22	1.73	0.69
1:A:696:GLU:CG	1:B:328:ARG:HG3	2.23	0.69
1:A:700:GLN:O	1:A:704:GLU:HG3	1.91	0.69
1:B:565:LEU:N	1:B:566:PRO:HD2	2.08	0.69
1:A:313:MET:CE	1:A:397:GLU:HA	2.23	0.69
1:A:671:LEU:HD23	1:A:671:LEU:N	2.08	0.69
1:A:696:GLU:HG2	1:B:328:ARG:HG3	1.74	0.69
1:B:282:LEU:O	1:B:348:LEU:HG	1.93	0.69
1:B:313:MET:CE	1:B:397:GLU:HA	2.23	0.69
1:B:665:ILE:CD1	1:B:666:GLN:N	2.55	0.69
1:A:306:ASN:ND2	1:A:308:THR:H	1.90	0.69
1:B:589:TYR:HB2	1:B:591:ILE:HG22	1.73	0.69
1:A:576:MET:HA	1:A:604:MET:CE	2.23	0.68
1:B:365:GLY:O	1:B:366:LYS:HG3	1.93	0.68
1:A:742:ILE:HG12	1:A:742:ILE:O	1.94	0.68
1:B:301:ILE:HD13	1:B:377:ARG:HG2	1.75	0.68
1:B:306:ASN:ND2	1:B:308:THR:H	1.91	0.68
1:A:282:LEU:O	1:A:348:LEU:HG	1.94	0.68
1:B:742:ILE:HG12	1:B:742:ILE:O	1.94	0.68
1:A:291:SER:OG	1:A:366:LYS:HD2	1.93	0.68
1:B:421:GLU:HG2	1:B:493:LEU:HD13	1.75	0.68
1:A:365:GLY:O	1:A:366:LYS:HG3	1.94	0.67
1:A:301:ILE:HD13	1:A:377:ARG:HG2	1.76	0.67
1:B:671:LEU:HD23	1:B:671:LEU:N	2.09	0.67
1:B:526:ALA:HB3	1:B:527:PRO:CD	2.21	0.67
1:A:328:ARG:HG3	1:B:696:GLU:CG	2.23	0.67
1:B:576:MET:HA	1:B:604:MET:CE	2.24	0.67
1:A:603:THR:HG22	1:A:606:GLU:OE1	1.94	0.67
1:B:291:SER:OG	1:B:366:LYS:HD2	1.95	0.67
1:B:492:ARG:HH11	1:B:492:ARG:HB2	1.60	0.67
1:A:341:LEU:O	1:A:342:GLU:HG2	1.95	0.67
1:B:603:THR:HG22	1:B:606:GLU:OE1	1.94	0.67
1:A:394:ARG:O	1:A:397:GLU:HB3	1.96	0.66
1:A:421:GLU:HG2	1:A:493:LEU:HD13	1.76	0.66
1:A:645:GLN:HE22	1:A:694:LYS:HG2	1.60	0.66
1:B:307:ARG:HH11	1:B:385:TYR:HD1	1.42	0.66
1:A:300:THR:C	1:A:302:PRO:HD2	2.15	0.66
1:B:341:LEU:O	1:B:342:GLU:HG2	1.95	0.66
1:A:434:LEU:HD21	1:A:438:ARG:NH2	2.09	0.66
1:B:389:LEU:O	1:B:393:ILE:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:NE2	1:A:359:ALA:HB1	2.11	0.66
1:A:517:LEU:HB3	1:A:582:VAL:HG22	1.78	0.66
1:B:360:PHE:CD2	1:B:362:PRO:HD3	2.30	0.66
1:A:441:LEU:HD13	1:A:504:LEU:HB3	1.77	0.66
1:A:360:PHE:CD2	1:A:362:PRO:HD3	2.30	0.66
1:A:469:ASN:ND2	1:A:480:ASN:HD21	1.91	0.66
1:A:389:LEU:O	1:A:393:ILE:HG12	1.96	0.65
1:B:300:THR:C	1:B:302:PRO:HD2	2.16	0.65
1:B:394:ARG:O	1:B:397:GLU:HB3	1.96	0.65
1:A:565:LEU:N	1:A:566:PRO:HD2	2.11	0.65
1:A:685:ILE:HG13	1:A:731:ILE:HD13	1.78	0.65
1:A:328:ARG:HG3	1:B:696:GLU:HG2	1.77	0.65
1:A:307:ARG:HH11	1:A:385:TYR:HD1	1.43	0.65
1:B:349:GLN:NE2	1:B:359:ALA:HB1	2.11	0.65
1:B:685:ILE:HG13	1:B:731:ILE:HD13	1.79	0.65
1:B:376:GLN:HE21	1:B:376:GLN:HA	1.61	0.65
1:A:436:GLU:O	1:A:440:LEU:HG	1.96	0.65
1:B:645:GLN:HE22	1:B:694:LYS:HG2	1.62	0.65
1:B:434:LEU:HD21	1:B:438:ARG:NH2	2.11	0.65
1:A:685:ILE:HG13	1:A:731:ILE:CD1	2.27	0.64
1:B:469:ASN:ND2	1:B:480:ASN:HD21	1.90	0.64
1:A:301:ILE:N	1:A:302:PRO:HD2	2.13	0.64
1:B:685:ILE:HG13	1:B:731:ILE:CD1	2.28	0.64
1:B:575:ILE:HG22	1:B:604:MET:CE	2.28	0.64
1:B:441:LEU:HD13	1:B:504:LEU:HB3	1.78	0.64
1:A:376:GLN:HE21	1:A:376:GLN:HA	1.62	0.63
1:B:517:LEU:HB3	1:B:582:VAL:HG22	1.80	0.63
1:A:526:ALA:HB3	1:A:527:PRO:CD	2.23	0.63
1:A:575:ILE:HG22	1:A:604:MET:CE	2.29	0.63
1:B:279:ASN:ND2	1:B:352:LEU:HD21	2.14	0.63
1:A:320:LEU:HA	1:A:389:LEU:HD13	1.81	0.63
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.63	0.63
1:A:492:ARG:HH11	1:A:492:ARG:HB2	1.63	0.62
1:A:706:LEU:HD11	1:B:317:GLN:HE22	1.64	0.62
1:B:286:TYR:OH	1:B:368:VAL:HG22	1.99	0.62
1:B:345:PHE:O	1:B:345:PHE:CG	2.52	0.62
1:A:305:GLU:HA	1:A:307:ARG:NH2	2.15	0.62
1:A:317:GLN:HE22	1:B:706:LEU:HD11	1.65	0.62
1:B:320:LEU:HA	1:B:389:LEU:HD13	1.81	0.62
1:B:297:ILE:O	1:B:301:ILE:HG13	2.00	0.62
1:B:301:ILE:N	1:B:302:PRO:HD2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:HG2	1:A:389:LEU:HD21	1.82	0.62
1:A:564:THR:C	1:A:566:PRO:HD2	2.21	0.61
1:A:592:ARG:HG2	1:A:592:ARG:HH11	1.65	0.61
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.65	0.61
1:A:469:ASN:HD21	1:A:480:ASN:ND2	1.96	0.61
1:A:279:ASN:ND2	1:A:352:LEU:HD21	2.14	0.61
1:B:564:THR:C	1:B:566:PRO:HD2	2.20	0.61
1:B:319:LYS:HG2	1:B:389:LEU:HD21	1.82	0.61
1:A:286:TYR:OH	1:A:368:VAL:HG22	2.01	0.61
1:A:556:THR:O	1:A:560:GLN:HG3	2.01	0.61
1:B:290:ALA:HB3	1:B:366:LYS:NZ	2.16	0.61
1:A:279:ASN:HD21	1:A:352:LEU:CD2	2.14	0.60
1:A:290:ALA:HB3	1:A:366:LYS:NZ	2.16	0.60
1:A:345:PHE:CG	1:A:345:PHE:O	2.53	0.60
1:B:665:ILE:HD12	1:B:666:GLN:N	2.16	0.60
1:A:297:ILE:O	1:A:301:ILE:HG13	2.01	0.60
1:B:517:LEU:HB3	1:B:582:VAL:CG2	2.31	0.60
1:A:735:ILE:O	1:A:739:GLU:HG3	2.00	0.60
1:A:665:ILE:HD12	1:A:666:GLN:N	2.15	0.60
1:A:463:ALA:O	1:A:466:GLN:HB3	2.01	0.60
1:A:639:ARG:HD3	1:A:709:ASP:O	2.01	0.60
1:B:279:ASN:HD21	1:B:352:LEU:CD2	2.14	0.60
1:B:305:GLU:HA	1:B:307:ARG:NH2	2.15	0.60
1:B:592:ARG:HG2	1:B:592:ARG:HH11	1.66	0.60
1:A:517:LEU:HB3	1:A:582:VAL:CG2	2.30	0.60
1:A:694:LYS:HB2	1:A:694:LYS:HZ2	1.67	0.60
1:B:436:GLU:O	1:B:440:LEU:HG	2.01	0.60
1:B:735:ILE:O	1:B:739:GLU:HG3	2.01	0.60
1:A:317:GLN:HB3	1:A:393:ILE:HD12	1.84	0.60
1:B:556:THR:O	1:B:560:GLN:HG3	2.02	0.60
1:A:575:ILE:HG22	1:A:604:MET:HE1	1.84	0.59
1:A:376:GLN:HA	1:A:376:GLN:NE2	2.17	0.59
1:B:339:CYS:O	1:B:341:LEU:O	2.21	0.59
1:B:317:GLN:HB3	1:B:393:ILE:HD12	1.83	0.59
1:B:576:MET:CA	1:B:604:MET:HE1	2.32	0.59
1:A:283:MET:HB2	1:A:360:PHE:CZ	2.38	0.59
1:A:341:LEU:C	1:A:343:ILE:H	2.06	0.59
1:A:350:THR:HA	1:A:353:ARG:CZ	2.33	0.58
1:B:283:MET:HB2	1:B:360:PHE:CZ	2.38	0.58
1:B:341:LEU:C	1:B:343:ILE:H	2.06	0.58
1:B:463:ALA:O	1:B:466:GLN:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:HE21	1:A:516:GLN:CA	2.16	0.58
1:B:516:GLN:HA	1:B:516:GLN:NE2	2.18	0.58
1:B:376:GLN:HA	1:B:376:GLN:NE2	2.17	0.58
1:B:469:ASN:HD21	1:B:480:ASN:ND2	1.94	0.58
1:A:339:CYS:O	1:A:341:LEU:O	2.21	0.58
1:B:350:THR:HA	1:B:353:ARG:CZ	2.33	0.58
1:B:516:GLN:HE21	1:B:516:GLN:CA	2.16	0.58
1:B:284:GLU:O	1:B:288:ARG:HG2	2.04	0.57
1:B:273:SER:O	1:B:277:GLN:HG3	2.05	0.57
1:B:432:ALA:HB3	1:B:437:VAL:HG23	1.86	0.57
1:A:432:ALA:HB3	1:A:437:VAL:HG23	1.85	0.57
1:A:273:SER:O	1:A:277:GLN:HG3	2.05	0.57
1:A:516:GLN:HA	1:A:516:GLN:NE2	2.19	0.57
1:A:284:GLU:O	1:A:288:ARG:HG2	2.05	0.57
1:B:643:ALA:HB1	1:B:712:HIS:O	2.05	0.57
1:B:434:LEU:O	1:B:438:ARG:HB2	2.05	0.56
1:A:370:ASP:C	1:A:372:ALA:N	2.60	0.55
1:A:441:LEU:HD13	1:A:504:LEU:CB	2.35	0.55
1:A:282:LEU:HB3	1:A:348:LEU:HD23	1.89	0.55
1:B:639:ARG:HD3	1:B:709:ASP:O	2.06	0.55
1:A:370:ASP:C	1:A:372:ALA:H	2.10	0.55
1:B:441:LEU:HD13	1:B:504:LEU:CB	2.36	0.55
1:B:518:HIS:HA	1:B:597:ASN:HD21	1.72	0.55
1:B:694:LYS:HB2	1:B:694:LYS:HZ3	1.71	0.55
1:A:669:GLY:O	1:A:670:ALA:O	2.25	0.55
1:A:354:ILE:HG22	1:A:354:ILE:O	2.07	0.55
1:B:469:ASN:O	1:B:472:ASP:N	2.39	0.55
1:A:434:LEU:O	1:A:438:ARG:HB2	2.07	0.55
1:A:643:ALA:HB1	1:A:712:HIS:O	2.07	0.55
1:A:662:ARG:O	1:A:664:SER:N	2.38	0.55
1:B:354:ILE:HG22	1:B:354:ILE:O	2.07	0.55
1:B:539:LEU:HD23	1:B:617:LEU:CB	2.37	0.55
1:A:518:HIS:HA	1:A:597:ASN:HD21	1.72	0.55
1:B:662:ARG:O	1:B:664:SER:N	2.40	0.54
1:A:350:THR:HA	1:A:353:ARG:NH2	2.22	0.54
1:A:342:GLU:CA	1:A:345:PHE:HB3	2.34	0.54
1:A:601:THR:HG23	1:B:443:LYS:HE2	1.89	0.54
1:B:282:LEU:HB3	1:B:348:LEU:HD23	1.89	0.54
1:B:410:ALA:HA	1:B:461:ILE:HD13	1.88	0.54
1:A:539:LEU:HD23	1:A:617:LEU:CB	2.37	0.54
1:A:390:LEU:HB3	1:A:394:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASN:ND2	1:A:659:GLU:OE2	2.41	0.54
1:B:370:ASP:C	1:B:372:ALA:N	2.60	0.54
1:B:370:ASP:C	1:B:372:ALA:H	2.10	0.54
1:B:532:MET:O	1:B:536:MET:HG3	2.06	0.54
1:B:585:VAL:O	1:B:589:TYR:HD2	1.91	0.54
1:A:301:ILE:N	1:A:302:PRO:CD	2.70	0.54
1:B:350:THR:HA	1:B:353:ARG:NH2	2.22	0.54
1:B:744:THR:O	1:B:744:THR:HG22	2.08	0.54
1:A:438:ARG:HD2	1:A:508:GLU:OE2	2.07	0.54
1:A:443:LYS:HE2	1:B:601:THR:HG23	1.89	0.54
1:B:301:ILE:N	1:B:302:PRO:CD	2.71	0.54
1:B:575:ILE:HG22	1:B:604:MET:HE2	1.88	0.53
1:B:342:GLU:CA	1:B:345:PHE:HB3	2.34	0.53
1:B:592:ARG:O	1:B:593:ILE:HB	2.08	0.53
1:B:566:PRO:HG2	1:B:567:GLU:H	1.73	0.53
1:A:324:ARG:NH1	1:B:703:GLN:OE1	2.41	0.53
1:A:410:ALA:HA	1:A:461:ILE:HD13	1.90	0.53
1:B:591:ILE:HG12	1:B:592:ARG:O	2.09	0.53
1:A:521:PHE:HE2	1:A:604:MET:HE2	1.74	0.53
1:B:438:ARG:HD2	1:B:508:GLU:OE2	2.08	0.53
1:A:585:VAL:O	1:A:589:TYR:HD2	1.90	0.53
1:B:669:GLY:O	1:B:670:ALA:O	2.26	0.53
1:A:280:GLU:HA	1:A:283:MET:HG2	1.91	0.53
1:A:363:SER:HB2	1:A:366:LYS:HB2	1.91	0.53
1:B:312:THR:O	1:B:396:LEU:HD13	2.09	0.53
1:B:363:SER:HB2	1:B:366:LYS:HB2	1.91	0.53
1:B:468:LEU:HG	1:B:473:TYR:CD1	2.45	0.52
1:B:410:ALA:HA	1:B:461:ILE:CD1	2.38	0.52
1:A:576:MET:CA	1:A:604:MET:HE1	2.37	0.52
1:A:536:MET:HE3	1:A:613:LYS:HB3	1.92	0.52
1:B:280:GLU:HA	1:B:283:MET:HG2	1.91	0.52
1:B:655:ASN:ND2	1:B:659:GLU:OE2	2.42	0.52
1:B:390:LEU:HB3	1:B:394:ARG:HH12	1.73	0.52
1:A:432:ALA:CB	1:A:437:VAL:HG23	2.40	0.52
1:A:566:PRO:HG2	1:A:567:GLU:H	1.74	0.52
1:B:304:LEU:C	1:B:306:ASN:H	2.13	0.52
1:B:516:GLN:NE2	1:B:516:GLN:CA	2.73	0.52
1:A:312:THR:O	1:A:396:LEU:HD13	2.10	0.52
1:B:316:MET:HE3	1:B:392:GLU:HG3	1.92	0.52
1:B:575:ILE:HG22	1:B:604:MET:HE1	1.90	0.52
1:B:634:ALA:HA	1:B:637:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASN:O	1:A:472:ASP:N	2.40	0.51
1:A:584:LYS:HD2	1:A:584:LYS:C	2.31	0.51
1:A:316:MET:HE3	1:A:392:GLU:HG3	1.92	0.51
1:A:591:ILE:HG12	1:A:592:ARG:O	2.10	0.51
1:A:304:LEU:C	1:A:306:ASN:H	2.12	0.51
1:A:592:ARG:O	1:A:593:ILE:HB	2.09	0.51
1:A:367:MET:CB	1:A:370:ASP:HB2	2.38	0.51
1:A:539:LEU:HD23	1:A:617:LEU:HB2	1.91	0.51
1:B:584:LYS:HD2	1:B:584:LYS:C	2.31	0.51
1:A:703:GLN:OE1	1:B:324:ARG:NH1	2.43	0.51
1:A:532:MET:O	1:A:536:MET:HG3	2.10	0.51
1:A:516:GLN:CA	1:A:516:GLN:NE2	2.73	0.51
1:A:544:ILE:HG23	1:A:544:ILE:O	2.10	0.51
1:A:634:ALA:HA	1:A:637:ARG:NH2	2.26	0.51
1:A:744:THR:HG22	1:A:744:THR:O	2.09	0.51
1:A:399:LEU:HD13	1:A:471:LEU:HB3	1.92	0.50
1:A:548:ILE:O	1:A:552:GLN:HG3	2.11	0.50
1:A:642:PHE:CE1	1:A:695:LEU:HD22	2.46	0.50
1:B:282:LEU:HB3	1:B:348:LEU:CD2	2.42	0.50
1:A:410:ALA:HA	1:A:461:ILE:CD1	2.42	0.50
1:B:642:PHE:CE1	1:B:695:LEU:HD22	2.47	0.50
1:B:733:ARG:HG3	1:B:733:ARG:HH11	1.77	0.50
1:A:733:ARG:HH11	1:A:733:ARG:HG3	1.76	0.50
1:A:297:ILE:HD12	1:A:297:ILE:C	2.32	0.50
1:A:543:PHE:HE1	1:A:628:GLU:HG3	1.77	0.50
1:B:394:ARG:HG3	1:B:394:ARG:NH1	2.27	0.50
1:B:489:GLN:HG2	1:B:493:LEU:HD22	1.94	0.50
1:B:623:GLN:O	1:B:627:GLU:HG3	2.12	0.50
1:B:273:SER:HA	1:B:276:ASN:ND2	2.25	0.50
1:A:457:ARG:O	1:A:461:ILE:HG13	2.12	0.49
1:A:489:GLN:HG2	1:A:493:LEU:HD22	1.93	0.49
1:B:399:LEU:HD13	1:B:471:LEU:HB3	1.93	0.49
1:A:506:ARG:HG3	1:A:506:ARG:HH11	1.76	0.49
1:B:548:ILE:O	1:B:552:GLN:HG3	2.12	0.49
1:A:737:GLU:O	1:A:741:GLN:NE2	2.45	0.49
1:B:594:SER:O	1:B:596:SER:N	2.46	0.49
1:B:694:LYS:O	1:B:695:LEU:C	2.51	0.49
1:A:623:GLN:O	1:A:627:GLU:HG3	2.13	0.49
1:B:307:ARG:NH1	1:B:385:TYR:HB2	2.27	0.49
1:A:348:LEU:HD12	1:A:360:PHE:CE1	2.47	0.49
1:A:350:THR:HA	1:A:353:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD12	1:B:360:PHE:CE1	2.47	0.49
1:B:506:ARG:HG3	1:B:506:ARG:HH11	1.77	0.49
1:A:380:GLN:O	1:A:383:LYS:HB2	2.13	0.49
1:A:468:LEU:HG	1:A:473:TYR:CD1	2.48	0.49
1:A:282:LEU:HB3	1:A:348:LEU:CD2	2.41	0.49
1:A:615:LYS:O	1:A:619:PRO:HD2	2.12	0.49
1:B:615:LYS:O	1:B:619:PRO:HD2	2.12	0.49
1:B:421:GLU:HG2	1:B:493:LEU:CD1	2.42	0.49
1:B:521:PHE:HE2	1:B:604:MET:HE2	1.78	0.49
1:A:273:SER:HA	1:A:276:ASN:ND2	2.25	0.49
1:B:297:ILE:C	1:B:297:ILE:HD12	2.33	0.49
1:B:492:ARG:O	1:B:496:LEU:HB2	2.12	0.49
1:A:307:ARG:NH1	1:A:385:TYR:HB2	2.28	0.48
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.28	0.48
1:B:517:LEU:CB	1:B:582:VAL:HG22	2.43	0.48
1:A:352:LEU:HD12	1:A:359:ALA:HA	1.95	0.48
1:A:492:ARG:O	1:A:496:LEU:HB2	2.13	0.48
1:B:367:MET:CB	1:B:370:ASP:HB2	2.38	0.48
1:B:539:LEU:HD23	1:B:617:LEU:HB2	1.94	0.48
1:B:733:ARG:O	1:B:737:GLU:HG3	2.14	0.48
1:A:662:ARG:C	1:A:664:SER:H	2.17	0.48
1:B:294:LEU:HD21	1:B:371:ILE:HG12	1.94	0.48
1:B:295:GLU:O	1:B:298:ARG:HB3	2.13	0.48
1:B:348:LEU:HD12	1:B:360:PHE:HE1	1.77	0.48
1:B:350:THR:HA	1:B:353:ARG:NH1	2.28	0.48
1:B:543:PHE:HE1	1:B:628:GLU:HG3	1.79	0.48
1:B:675:MET:HE2	1:B:738:VAL:HG12	1.95	0.48
1:B:380:GLN:O	1:B:383:LYS:HB2	2.13	0.48
1:A:741:GLN:C	1:A:743:LEU:H	2.17	0.48
1:B:352:LEU:HD12	1:B:359:ALA:HA	1.95	0.48
1:A:294:LEU:HD21	1:A:371:ILE:HG12	1.95	0.48
1:A:295:GLU:O	1:A:298:ARG:HB3	2.14	0.48
1:A:348:LEU:HD12	1:A:360:PHE:HE1	1.78	0.48
1:B:662:ARG:C	1:B:664:SER:H	2.16	0.48
1:A:594:SER:O	1:A:596:SER:N	2.46	0.47
1:A:575:ILE:HG22	1:A:604:MET:HE2	1.96	0.47
1:A:675:MET:HE2	1:A:738:VAL:HG12	1.96	0.47
1:B:427:LYS:O	1:B:429:TYR:N	2.47	0.47
1:A:427:LYS:O	1:A:429:TYR:N	2.48	0.47
1:A:517:LEU:CB	1:A:582:VAL:HG22	2.42	0.47
1:B:281:ARG:HG3	1:B:282:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:TRP:HE3	1:B:304:LEU:HD22	1.80	0.47
1:A:733:ARG:O	1:A:737:GLU:HG3	2.14	0.47
1:B:432:ALA:CB	1:B:437:VAL:HG23	2.44	0.47
1:B:737:GLU:O	1:B:741:GLN:NE2	2.47	0.47
1:A:303:TRP:HE3	1:A:304:LEU:HD22	1.80	0.47
1:B:544:ILE:HG23	1:B:544:ILE:O	2.15	0.47
1:A:696:GLU:HG2	1:B:328:ARG:CG	2.44	0.47
1:A:715:TYR:C	1:A:716:THR:HG23	2.35	0.47
1:B:589:TYR:O	1:B:590:ASN:C	2.53	0.47
1:A:417:ALA:O	1:A:418:TYR:C	2.53	0.47
1:B:304:LEU:HD22	1:B:304:LEU:N	2.30	0.47
1:A:304:LEU:HD22	1:A:304:LEU:N	2.30	0.47
1:A:281:ARG:HG3	1:A:282:LEU:CD1	2.45	0.46
1:B:526:ALA:CB	1:B:527:PRO:HD3	2.26	0.46
1:B:585:VAL:CG2	1:B:586:ILE:N	2.78	0.46
1:B:715:TYR:O	1:B:716:THR:HG23	2.15	0.46
1:B:496:LEU:HD12	1:B:496:LEU:HA	1.74	0.46
1:B:741:GLN:C	1:B:743:LEU:H	2.18	0.46
1:A:589:TYR:O	1:A:590:ASN:C	2.53	0.46
1:A:318:LYS:HD2	1:A:318:LYS:O	2.15	0.46
1:A:585:VAL:CG2	1:A:586:ILE:N	2.78	0.46
1:A:706:LEU:HD11	1:B:317:GLN:NE2	2.30	0.46
1:A:278:GLU:CA	1:A:281:ARG:HG2	2.43	0.46
1:B:715:TYR:C	1:B:716:THR:HG23	2.36	0.46
1:B:313:MET:HE3	1:B:397:GLU:HA	1.98	0.46
1:B:417:ALA:O	1:B:418:TYR:C	2.52	0.46
1:A:464:ILE:O	1:A:468:LEU:HB2	2.16	0.45
1:A:585:VAL:HG23	1:A:586:ILE:N	2.32	0.45
1:B:304:LEU:O	1:B:306:ASN:N	2.49	0.45
1:A:304:LEU:HD22	1:A:304:LEU:H	1.81	0.45
1:A:304:LEU:O	1:A:306:ASN:N	2.48	0.45
1:A:545:VAL:CG1	1:A:550:GLU:HB3	2.47	0.45
1:B:346:ASN:HA	1:B:349:GLN:HB2	1.99	0.45
1:B:518:HIS:HA	1:B:597:ASN:ND2	2.31	0.45
1:A:340:GLN:O	1:A:343:ILE:HB	2.17	0.45
1:B:304:LEU:HD22	1:B:304:LEU:H	1.82	0.45
1:B:357:ARG:O	1:B:357:ARG:CG	2.60	0.45
1:A:565:LEU:N	1:A:566:PRO:CD	2.80	0.45
1:B:335:VAL:HG22	1:B:375:TRP:CZ2	2.51	0.45
1:B:457:ARG:O	1:B:461:ILE:HG13	2.17	0.45
1:A:421:GLU:HG2	1:A:493:LEU:CD1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:TYR:O	1:A:716:THR:HG23	2.16	0.45
1:A:548:ILE:HD13	1:A:633:HIS:CE1	2.52	0.44
1:B:565:LEU:N	1:B:566:PRO:CD	2.77	0.44
1:A:335:VAL:HG22	1:A:375:TRP:CZ2	2.52	0.44
1:B:545:VAL:CG1	1:B:550:GLU:HB3	2.48	0.44
1:A:346:ASN:HA	1:A:349:GLN:HB2	1.99	0.44
1:B:278:GLU:CA	1:B:281:ARG:HG2	2.43	0.44
1:B:340:GLN:O	1:B:343:ILE:HB	2.16	0.44
1:B:576:MET:N	1:B:604:MET:HE1	2.32	0.44
1:A:296:TRP:C	1:A:298:ARG:N	2.71	0.44
1:B:402:LEU:HB3	1:B:468:LEU:HD13	2.00	0.44
1:B:296:TRP:C	1:B:298:ARG:N	2.71	0.44
1:A:576:MET:N	1:A:604:MET:HE1	2.33	0.44
1:A:518:HIS:HA	1:A:597:ASN:ND2	2.33	0.44
1:A:357:ARG:O	1:A:357:ARG:CG	2.61	0.44
1:A:427:LYS:O	1:A:428:ASP:C	2.57	0.44
1:A:639:ARG:NH1	1:A:709:ASP:OD1	2.51	0.44
1:B:318:LYS:HD2	1:B:318:LYS:O	2.18	0.44
1:B:639:ARG:HG2	1:B:710:ASN:CG	2.38	0.44
1:A:419:GLY:O	1:A:423:ILE:HG23	2.18	0.43
1:A:594:SER:C	1:A:596:SER:N	2.71	0.43
1:B:585:VAL:O	1:B:589:TYR:CD2	2.71	0.43
1:B:585:VAL:HG23	1:B:586:ILE:N	2.32	0.43
1:A:589:TYR:HB2	1:A:591:ILE:CG2	2.45	0.43
1:B:423:ILE:HD12	1:B:423:ILE:O	2.18	0.43
1:A:371:ILE:HG22	1:A:371:ILE:O	2.19	0.43
1:A:743:LEU:HD12	1:B:354:ILE:CD1	2.48	0.43
1:B:743:LEU:C	1:B:745:ARG:H	2.22	0.43
1:A:639:ARG:HG2	1:A:710:ASN:CG	2.39	0.43
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.87	0.43
1:B:625:LEU:HD12	1:B:625:LEU:HA	1.90	0.43
1:A:296:TRP:HA	1:A:299:ARG:HG2	2.00	0.43
1:A:313:MET:HB2	1:A:396:LEU:HB3	2.01	0.43
1:A:328:ARG:CG	1:B:696:GLU:HG2	2.46	0.43
1:B:290:ALA:HB3	1:B:366:LYS:HZ1	1.84	0.43
1:B:427:LYS:O	1:B:428:ASP:C	2.57	0.43
1:B:357:ARG:O	1:B:358:PRO:C	2.57	0.43
1:B:514:ILE:HD13	1:B:586:ILE:HG12	2.01	0.43
1:A:357:ARG:O	1:A:358:PRO:C	2.57	0.43
1:B:408:GLN:O	1:B:412:THR:HG23	2.19	0.43
1:A:585:VAL:O	1:A:589:TYR:CD2	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:GLN:HG3	1:B:583:GLU:OE2	2.19	0.43
1:A:352:LEU:CD1	1:A:359:ALA:HA	2.49	0.43
1:B:613:LYS:O	1:B:614:VAL:C	2.56	0.43
1:A:303:TRP:CZ3	1:A:304:LEU:HD13	2.54	0.43
1:A:514:ILE:HD13	1:A:586:ILE:HG12	2.00	0.43
1:A:521:PHE:CE2	1:A:604:MET:HE2	2.53	0.43
1:A:670:ALA:HB1	1:A:671:LEU:H	1.65	0.43
1:A:743:LEU:HD12	1:B:354:ILE:HD12	2.01	0.43
1:B:303:TRP:CE3	1:B:304:LEU:HD13	2.54	0.43
1:B:309:PRO:HA	1:B:316:MET:HE1	2.01	0.43
1:B:313:MET:HB2	1:B:396:LEU:HB3	2.01	0.43
1:B:362:PRO:O	1:B:363:SER:C	2.57	0.43
1:B:532:MET:HE3	1:B:610:LYS:HB3	2.01	0.42
1:A:362:PRO:O	1:A:363:SER:C	2.58	0.42
1:B:433:SER:N	1:B:436:GLU:OE1	2.51	0.42
1:A:347:THR:O	1:A:347:THR:HG22	2.19	0.42
1:A:579:GLN:HG3	1:A:583:GLU:OE2	2.19	0.42
1:B:536:MET:CE	1:B:613:LYS:HB3	2.50	0.42
1:A:286:TYR:OH	1:A:368:VAL:HG13	2.20	0.42
1:B:352:LEU:CD1	1:B:359:ALA:HA	2.49	0.42
1:B:371:ILE:O	1:B:371:ILE:HG22	2.19	0.42
1:A:368:VAL:HG12	1:A:368:VAL:O	2.19	0.42
1:B:287:GLU:OE1	1:B:362:PRO:HB2	2.19	0.42
1:B:521:PHE:HE2	1:B:604:MET:CE	2.32	0.42
1:B:695:LEU:HD23	1:B:695:LEU:HA	1.84	0.42
1:A:715:TYR:O	1:A:716:THR:OG1	2.36	0.42
1:A:743:LEU:C	1:A:745:ARG:H	2.22	0.42
1:B:368:VAL:O	1:B:368:VAL:HG12	2.20	0.42
1:A:298:ARG:HG2	1:A:298:ARG:HH11	1.84	0.42
1:B:303:TRP:CZ3	1:B:304:LEU:HD13	2.54	0.42
1:B:594:SER:C	1:B:596:SER:N	2.72	0.42
1:A:287:GLU:OE1	1:A:362:PRO:HB2	2.20	0.42
1:A:493:LEU:HD12	1:A:493:LEU:HA	1.83	0.42
1:A:593:ILE:N	1:A:593:ILE:HD12	2.35	0.42
1:B:296:TRP:HA	1:B:299:ARG:HG2	2.00	0.42
1:B:347:THR:HG22	1:B:347:THR:O	2.20	0.42
1:B:450:ASP:O	1:B:453:ALA:HB3	2.20	0.42
1:B:451:LEU:C	1:B:451:LEU:HD13	2.40	0.42
1:B:603:THR:O	1:B:607:LEU:HB2	2.20	0.42
1:B:694:LYS:HB2	1:B:694:LYS:HZ2	1.85	0.42
1:A:307:ARG:HG3	1:A:388:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:PRO:HA	1:A:316:MET:HE1	2.02	0.42
1:A:423:ILE:HD12	1:A:423:ILE:O	2.20	0.42
1:B:319:LYS:CG	1:B:389:LEU:HD21	2.49	0.42
1:B:376:GLN:NE2	1:B:376:GLN:CA	2.79	0.42
1:A:294:LEU:O	1:A:297:ILE:HG13	2.20	0.41
1:A:303:TRP:CE3	1:A:304:LEU:HD13	2.54	0.41
1:A:536:MET:CE	1:A:613:LYS:HB3	2.50	0.41
1:A:733:ARG:CZ	1:A:733:ARG:HB2	2.50	0.41
1:B:286:TYR:OH	1:B:368:VAL:HG13	2.20	0.41
1:A:317:GLN:NE2	1:B:706:LEU:HD11	2.31	0.41
1:A:350:THR:CG2	1:A:353:ARG:HH12	2.19	0.41
1:A:715:TYR:O	1:A:716:THR:CB	2.68	0.41
1:B:307:ARG:HG3	1:B:388:TRP:CD2	2.56	0.41
1:B:526:ALA:CB	1:B:527:PRO:CD	2.91	0.41
1:B:536:MET:HE3	1:B:613:LYS:HB3	2.02	0.41
1:A:281:ARG:HG3	1:A:282:LEU:HD12	2.03	0.41
1:A:694:LYS:O	1:A:695:LEU:C	2.56	0.41
1:B:641:GLN:O	1:B:645:GLN:HG3	2.21	0.41
1:B:715:TYR:O	1:B:716:THR:CB	2.69	0.41
1:B:716:THR:O	1:B:717:MET:C	2.59	0.41
1:A:506:ARG:HG3	1:A:506:ARG:NH1	2.34	0.41
1:B:296:TRP:CE3	1:B:334:LYS:HG2	2.56	0.41
1:B:301:ILE:HG12	1:B:378:LEU:HA	2.03	0.41
1:B:356:ASN:O	1:B:357:ARG:HB3	2.20	0.41
1:A:319:LYS:CG	1:A:389:LEU:HD21	2.49	0.41
1:A:603:THR:O	1:A:607:LEU:HB2	2.20	0.41
1:B:733:ARG:O	1:B:736:ASN:HB3	2.21	0.41
1:A:296:TRP:CE3	1:A:334:LYS:HG2	2.55	0.41
1:A:332:PRO:N	1:A:333:PRO:HD2	2.36	0.41
1:A:433:SER:N	1:A:436:GLU:OE1	2.50	0.41
1:A:508:GLU:O	1:A:512:GLU:HB2	2.21	0.41
1:B:434:LEU:CD2	1:B:438:ARG:NH2	2.81	0.41
1:B:506:ARG:HG3	1:B:506:ARG:NH1	2.35	0.41
1:B:562:LYS:HD3	1:B:618:VAL:CG1	2.50	0.41
1:B:361:MET:HA	1:B:362:PRO:HD2	1.91	0.41
1:B:656:LYS:CE	1:B:684:ASN:HD22	2.34	0.41
1:A:300:THR:O	1:A:304:LEU:HD23	2.21	0.41
1:A:316:MET:HE2	1:A:392:GLU:HB3	2.03	0.41
1:A:356:ASN:O	1:A:357:ARG:HB3	2.21	0.41
1:A:390:LEU:O	1:A:393:ILE:N	2.54	0.41
1:A:425:LEU:HD21	1:A:496:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASP:O	1:A:453:ALA:HB3	2.21	0.41
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.85	0.41
1:B:294:LEU:O	1:B:297:ILE:HG13	2.21	0.41
1:B:298:ARG:HH11	1:B:298:ARG:HG2	1.86	0.41
1:B:438:ARG:CD	1:B:508:GLU:OE2	2.69	0.41
1:B:671:LEU:O	1:B:674:GLN:N	2.53	0.41
1:A:301:ILE:HG12	1:A:378:LEU:HA	2.03	0.41
1:A:313:MET:HE3	1:A:397:GLU:HA	1.98	0.41
1:A:341:LEU:C	1:A:343:ILE:N	2.73	0.41
1:A:408:GLN:O	1:A:412:THR:HG23	2.21	0.41
1:A:619:PRO:O	1:A:623:GLN:HB2	2.21	0.41
1:B:281:ARG:HG3	1:B:282:LEU:HD12	2.03	0.41
1:B:302:PRO:O	1:B:304:LEU:O	2.40	0.41
1:B:303:TRP:C	1:B:304:LEU:O	2.57	0.41
1:B:589:TYR:HB2	1:B:591:ILE:CG2	2.44	0.41
1:B:619:PRO:O	1:B:623:GLN:HB2	2.21	0.41
1:A:562:LYS:HD3	1:A:618:VAL:CG1	2.51	0.40
1:A:696:GLU:OE2	1:A:721:ARG:NH2	2.47	0.40
1:B:466:GLN:O	1:B:469:ASN:HB2	2.21	0.40
1:B:593:ILE:O	1:B:593:ILE:HG22	2.22	0.40
1:A:280:GLU:O	1:A:283:MET:HG2	2.21	0.40
1:A:308:THR:HA	1:A:309:PRO:HD2	1.89	0.40
1:A:434:LEU:CD2	1:A:438:ARG:NH2	2.81	0.40
1:B:508:GLU:O	1:B:512:GLU:HB2	2.21	0.40
1:A:641:GLN:O	1:A:645:GLN:HG3	2.22	0.40
1:A:438:ARG:CD	1:A:508:GLU:OE2	2.70	0.40
1:A:656:LYS:CE	1:A:684:ASN:HD22	2.35	0.40
1:B:276:ASN:O	1:B:280:GLU:HG3	2.22	0.40
1:B:300:THR:O	1:B:304:LEU:HD23	2.22	0.40
1:B:344:ASN:C	1:B:346:ASN:H	2.25	0.40
1:B:350:THR:CG2	1:B:353:ARG:HH12	2.19	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	473/476 (99%)	385 (81%)	64 (14%)	24 (5%)	2 6
1	B	473/476 (99%)	386 (82%)	62 (13%)	25 (5%)	2 6
All	All	946/952 (99%)	771 (82%)	126 (13%)	49 (5%)	2 6

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	SER
1	A	356	ASN
1	A	358	PRO
1	A	362	PRO
1	A	363	SER
1	A	383	LYS
1	A	428	ASP
1	A	665	ILE
1	A	670	ALA
1	B	355	SER
1	B	356	ASN
1	B	358	PRO
1	B	362	PRO
1	B	363	SER
1	B	383	LYS
1	B	428	ASP
1	B	665	ILE
1	B	670	ALA
1	A	309	PRO
1	A	311	LYS
1	A	359	ALA
1	A	595	SER
1	A	742	ILE
1	B	309	PRO
1	B	311	LYS
1	B	359	ALA
1	B	595	SER
1	B	742	ILE
1	A	306	ASN
1	A	367	MET
1	A	592	ARG
1	A	663	SER
1	A	666	GLN

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Mol	Chain	Res	Type
1	B	306	ASN
1	B	367	MET
1	B	592	ARG
1	B	663	SER
1	B	666	GLN
1	A	366	LYS
1	A	590	ASN
1	B	366	LYS
1	B	590	ASN
1	A	357	ARG
1	A	593	ILE
1	B	357	ARG
1	B	470	GLU
1	B	593	ILE
1	A	716	THR
1	B	716	THR

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	426/426 (100%)	390 (92%)	36 (8%)	10 31
1	B	426/426 (100%)	390 (92%)	36 (8%)	10 31
All	All	852/852 (100%)	780 (92%)	72 (8%)	10 31

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	LEU
1	A	295	GLU
1	A	314	GLN
1	A	320	LEU
1	A	328	ARG
1	A	348	LEU
1	A	358	PRO

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Mol	Chain	Res	Type
1	A	360	PHE
1	A	361	MET
1	A	370	ASP
1	A	407	ARG
1	A	420	LYS
1	A	423	ILE
1	A	438	ARG
1	A	468	LEU
1	A	479	VAL
1	A	493	LEU
1	A	516	GLN
1	A	567	GLU
1	A	584	LYS
1	A	587	GLN
1	A	591	ILE
1	A	592	ARG
1	A	601	THR
1	A	610	LYS
1	A	621	ARG
1	A	625	LEU
1	A	631	ARG
1	A	639	ARG
1	A	676	ASN
1	A	693	ASP
1	A	695	LEU
1	A	731	ILE
1	A	741	GLN
1	A	743	LEU
1	A	745	ARG
1	B	289	LEU
1	B	295	GLU
1	B	314	GLN
1	B	320	LEU
1	B	328	ARG
1	B	348	LEU
1	B	358	PRO
1	B	360	PHE
1	B	361	MET
1	B	370	ASP
1	B	407	ARG
1	B	420	LYS
1	B	423	ILE

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Mol	Chain	Res	Type
1	B	438	ARG
1	B	468	LEU
1	B	479	VAL
1	B	493	LEU
1	B	516	GLN
1	B	567	GLU
1	B	584	LYS
1	B	587	GLN
1	B	591	ILE
1	B	592	ARG
1	B	601	THR
1	B	610	LYS
1	B	621	ARG
1	B	625	LEU
1	B	631	ARG
1	B	639	ARG
1	B	676	ASN
1	B	693	ASP
1	B	695	LEU
1	B	731	ILE
1	B	741	GLN
1	B	743	LEU
1	B	745	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	306	ASN
1	A	317	GLN
1	A	349	GLN
1	A	376	GLN
1	A	408	GLN
1	A	426	GLN
1	A	480	ASN
1	A	516	GLN
1	A	530	ASN
1	A	540	GLN
1	A	579	GLN
1	A	580	ASN
1	A	587	GLN
1	A	616	GLN

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Mol	Chain	Res	Type
1	A	645	GLN
1	A	684	ASN
1	A	700	GLN
1	A	736	ASN
1	A	741	GLN
1	B	276	ASN
1	B	306	ASN
1	B	317	GLN
1	B	376	GLN
1	B	408	GLN
1	B	426	GLN
1	B	480	ASN
1	B	516	GLN
1	B	530	ASN
1	B	540	GLN
1	B	579	GLN
1	B	580	ASN
1	B	587	GLN
1	B	616	GLN
1	B	645	GLN
1	B	684	ASN
1	B	700	GLN
1	B	736	ASN
1	B	741	GLN

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	475/476 (99%)	0.50	24 (5%)	28	19	39, 64, 131, 156	0
1	B	475/476 (99%)	0.51	21 (4%)	34	24	33, 64, 132, 156	0
All	All	950/952 (99%)	0.50	45 (4%)	31	22	33, 64, 132, 156	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	VAL	7.4
1	A	359	ALA	6.7
1	B	282	LEU	6.6
1	A	368	VAL	6.4
1	A	282	LEU	4.3
1	B	359	ALA	4.0
1	A	361	MET	3.8
1	A	354	ILE	3.7
1	B	362	PRO	3.4
1	B	348	LEU	3.3
1	B	361	MET	3.3
1	B	354	ILE	3.1
1	A	352	LEU	3.0
1	B	289	LEU	3.0
1	B	293	LEU	2.9
1	B	278	GLU	2.9
1	A	348	LEU	2.8
1	A	378	LEU	2.8
1	A	595	SER	2.8
1	A	347	THR	2.8
1	A	289	LEU	2.7
1	A	670	ALA	2.6
1	B	367	MET	2.6
1	A	290	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	273	SER	2.5
1	A	366	LYS	2.5
1	B	347	THR	2.5
1	A	362	PRO	2.5
1	B	272	SER	2.5
1	A	345	PHE	2.5
1	A	360	PHE	2.4
1	B	352	LEU	2.3
1	A	665	ILE	2.3
1	A	286	TYR	2.3
1	B	378	LEU	2.2
1	A	341	LEU	2.2
1	A	407	ARG	2.2
1	B	604	MET	2.1
1	B	360	PHE	2.1
1	B	303	TRP	2.1
1	A	375	TRP	2.1
1	A	593	ILE	2.0
1	B	275	VAL	2.0
1	A	272	SER	2.0
1	B	355	SER	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 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.