Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 07:29 PM EDT

PDB ID	:	1N4M
Title	:	Structure of Rb tumor suppressor bound to the transactivation domain of E2F-2
Authors	:	Lee, C.; Chang, J.H.; Lee, H.S.; Cho, Y.
Deposited on	:	2002-10-31
Resolution	:	2.20 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 (i)) were used in the production of this report:

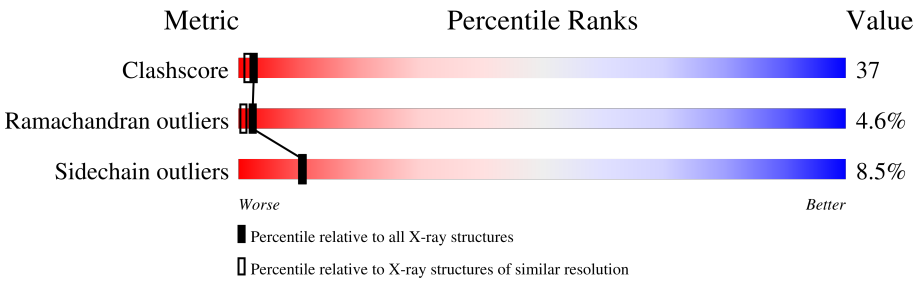
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	45% 44% 10% •
1	B	345	47% 45% 6% •
2	C	18	61% 33% 6%
2	D	18	39% 56% 6%
2	E	18	17% 17% 22% 11% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6249 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 Retinoblastoma Pocket.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	2829	1817	477	515	20	0	0	0
1	B	338	2780	1790	468	502	20	0	0	0

- Molecule 2 is a protein called Transcription factor E2F2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	18	143	91	19	33	0	0	0
2	D	18	143	91	19	33	0	0	0
2	E	12	93	59	13	21	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	144	144	144	0	0
3	B	100	100	100	0	0
3	C	4	4	4	0	0
3	D	6	6	6	0	0
3	E	7	7	7	0	0

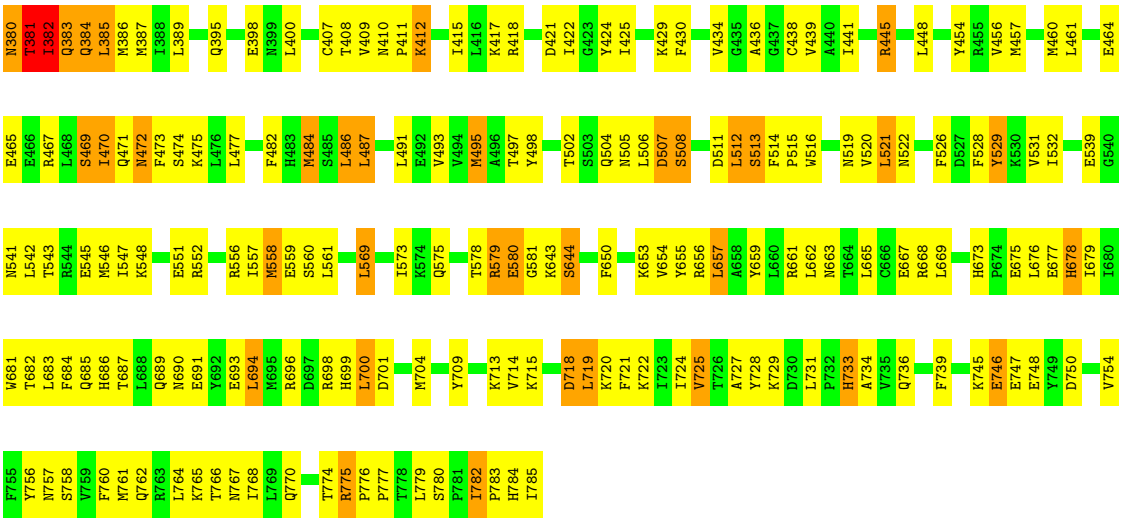
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

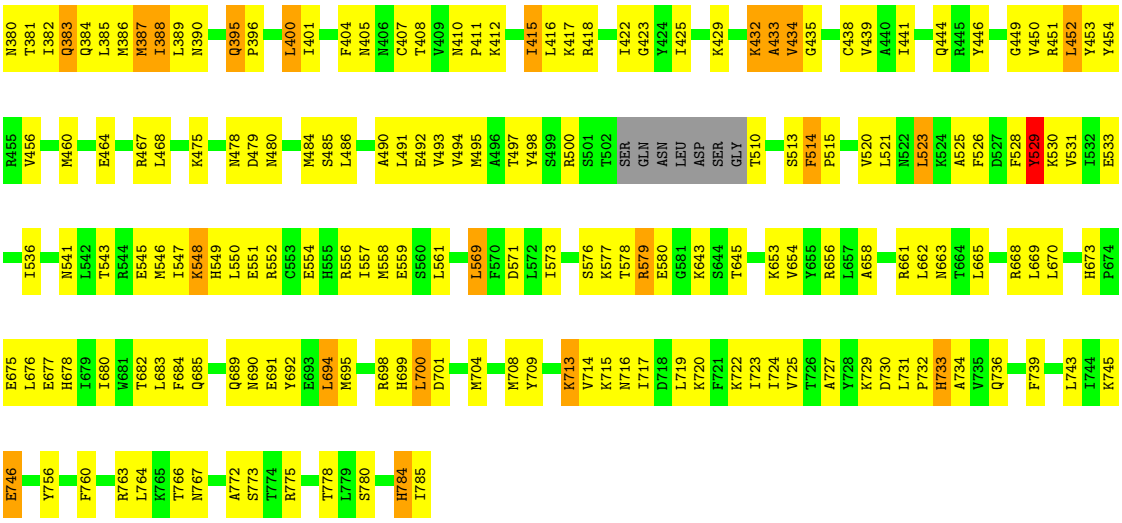
• Molecule 1: Retinoblastoma Pocket

Chain A: 45% 44% 10%



• Molecule 1: Retinoblastoma Pocket

Chain B: 47% 45% 6%

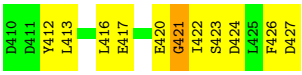


• Molecule 2: Transcription factor E2F2

Chain C:

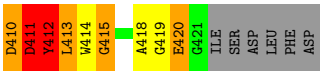
• Molecule 2: Transcription factor E2F2

Chain D:



• Molecule 2: Transcription factor E2F2

Chain E:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.37Å 65.16Å 69.34Å 85.55° 79.48° 67.16°	Depositor
Resolution (Å)	19.65 – 2.20	Depositor
% Data completeness (in resolution range)	85.5 (19.65-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6249	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

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	0.48	0/2885	0.67	0/3887
1	B	0.46	0/2835	0.64	0/3818
2	C	0.50	0/146	0.70	0/196
2	D	0.39	0/146	0.58	0/196
2	E	0.63	0/95	1.13	1/128 (0.8%)
All	All	0.47	0/6107	0.67	1/8225 (0.0%)

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	B	0	1

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	E	415	GLY	N-CA-C	-5.23	100.03	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	529	TYR	Sidechain

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	2829	0	2886	224	0
1	B	2780	0	2843	210	0
2	C	143	0	118	8	0
2	D	143	0	118	17	0
2	E	93	0	74	16	0
3	A	144	0	0	15	0
3	B	100	0	0	12	0
3	C	4	0	0	2	0
3	D	6	0	0	0	0
3	E	7	0	0	0	0
All	All	6249	0	6039	447	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 37.

All (447) 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:385:LEU:HD13	1:B:388:ILE:HD11	1.33	1.08
1:A:774:THR:HG23	1:A:775:ARG:HD3	1.36	1.04
1:B:552:ARG:HH12	1:B:733:HIS:HB3	1.24	0.99
1:A:643:LYS:HG2	1:A:644:SER:H	1.28	0.99
1:B:694:LEU:HD13	1:B:763:ARG:HH21	1.26	0.98
1:A:579:ARG:HH22	1:A:643:LYS:HD3	1.29	0.97
1:A:643:LYS:HG2	1:A:644:SER:N	1.79	0.97
1:B:385:LEU:HD21	1:B:541:ASN:O	1.69	0.93
1:B:745:LYS:NZ	1:B:746:GLU:HG2	1.82	0.92
1:A:729:LYS:NZ	1:A:736:GLN:HE21	1.70	0.90
1:A:460:MET:HE1	1:A:486:LEU:HD21	1.52	0.90
1:A:689:GLN:HG2	1:A:690:ASN:ND2	1.88	0.88
1:B:546:MET:HE3	1:B:549:HIS:HB3	1.58	0.86
1:A:784:HIS:O	1:A:785:ILE:HG13	1.74	0.85
1:A:668:ARG:HB2	1:A:668:ARG:NH1	1.92	0.85
1:A:685:GLN:HE22	1:A:689:GLN:NE2	1.74	0.85
1:B:745:LYS:HD2	1:B:746:GLU:N	1.92	0.84
1:B:745:LYS:HD2	1:B:746:GLU:H	1.42	0.84
1:B:554:GLU:O	1:B:558:MET:HG2	1.78	0.83
1:A:429:LYS:HD2	1:A:520:VAL:HG13	1.61	0.83
1:A:558:MET:HG3	1:A:654:VAL:HG22	1.58	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ARG:HG2	2:D:413:LEU:HB2	1.60	0.82
1:B:425:ILE:O	1:B:429:LYS:HG2	1.81	0.81
1:A:668:ARG:HB2	1:A:668:ARG:HH11	1.45	0.80
1:B:547:ILE:O	1:B:551:GLU:HG2	1.83	0.78
1:B:383:GLN:HE21	1:B:383:GLN:HA	1.47	0.78
1:A:505:ASN:HA	3:A:98:HOH:O	1.85	0.77
1:A:691:GLU:HG3	1:A:764:LEU:HD21	1.65	0.77
1:B:670:LEU:HD22	1:B:676:LEU:HD12	1.68	0.76
1:A:487:LEU:HD22	1:A:491:LEU:HD11	1.68	0.75
2:E:411:ASP:O	2:E:412:TYR:HB2	1.86	0.75
1:B:701:ASP:OD2	1:B:733:HIS:HD2	1.71	0.74
1:A:512:LEU:HD12	1:A:512:LEU:O	1.86	0.74
1:A:438:CYS:O	1:A:441:ILE:HG22	1.86	0.74
1:A:669:LEU:HD23	1:A:719:LEU:HD11	1.68	0.74
1:B:494:VAL:O	1:B:497:THR:HG22	1.88	0.74
1:B:429:LYS:O	1:B:433:ALA:HB3	1.88	0.74
1:B:773:SER:HB2	2:E:410:ASP:N	2.03	0.73
1:B:417:LYS:NZ	1:B:417:LYS:HB3	2.04	0.73
1:A:381:THR:HG23	1:A:384:GLN:HB2	1.69	0.73
1:A:729:LYS:HZ3	1:A:736:GLN:HE21	1.35	0.72
1:A:669:LEU:HD11	1:A:727:ALA:CB	2.20	0.72
1:B:475:LYS:HG2	2:D:427:ASP:OXT	1.89	0.72
1:A:766:THR:O	1:A:770:GLN:HG3	1.89	0.72
1:A:493:VAL:O	1:A:497:THR:HG23	1.90	0.72
1:A:673:HIS:HB3	1:A:675:GLU:OE2	1.89	0.72
1:B:385:LEU:HD13	1:B:388:ILE:CD1	2.16	0.72
1:B:380:ASN:HB3	1:B:541:ASN:ND2	2.05	0.71
1:B:395:GLN:HB2	1:B:396:PRO:HD2	1.71	0.71
1:A:557:ILE:HA	1:A:561:LEU:HB2	1.72	0.71
1:A:382:ILE:HD13	1:A:545:GLU:OE2	1.90	0.71
1:A:434:VAL:HG22	1:A:506:LEU:HD13	1.72	0.71
1:A:656:ARG:HG2	2:C:413:LEU:HB2	1.71	0.71
2:E:412:TYR:HE2	2:E:414:TRP:HE1	1.37	0.71
1:A:579:ARG:NH2	1:A:643:LYS:HD3	2.03	0.70
1:A:575:GLN:HG2	1:A:579:ARG:HH21	1.55	0.70
1:B:729:LYS:HE3	1:B:736:GLN:HG3	1.73	0.70
1:A:643:LYS:CG	1:A:644:SER:H	2.01	0.70
1:B:438:CYS:HB2	1:B:441:ILE:HD12	1.74	0.70
1:A:491:LEU:O	1:A:495:MET:HB2	1.91	0.69
1:B:698:ARG:HG2	3:B:170:HOH:O	1.91	0.69
1:B:467:ARG:HE	2:D:420:GLU:N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:GLU:HB2	1:B:699:HIS:CE1	2.27	0.69
1:A:762:GLN:HA	1:A:762:GLN:HE21	1.58	0.69
2:D:422:ILE:HD11	2:D:426:PHE:HE1	1.58	0.68
1:B:685:GLN:HE22	1:B:689:GLN:NE2	1.91	0.68
1:A:385:LEU:HD22	1:A:389:LEU:HG	1.75	0.68
1:A:663:ASN:O	1:A:667:GLU:HG2	1.94	0.67
1:B:656:ARG:NH2	1:B:785:ILE:HG23	2.09	0.67
1:A:575:GLN:HG2	1:A:579:ARG:HD2	1.77	0.67
1:B:417:LYS:HB3	1:B:417:LYS:HZ3	1.58	0.67
1:B:552:ARG:HH12	1:B:733:HIS:CB	2.03	0.67
1:A:425:ILE:HG23	1:A:429:LYS:HE2	1.76	0.66
1:A:558:MET:HE3	1:A:653:LYS:HB3	1.78	0.66
2:E:412:TYR:CE2	2:E:414:TRP:NE1	2.63	0.66
1:A:382:ILE:HD12	1:A:543:THR:HG21	1.77	0.66
2:E:412:TYR:HD2	2:E:414:TRP:CD1	2.14	0.66
1:B:678:HIS:HE1	1:B:780:SER:O	1.79	0.65
1:B:691:GLU:HG3	1:B:764:LEU:HD21	1.76	0.65
1:B:452:LEU:HB3	1:B:490:ALA:HB1	1.79	0.65
1:B:490:ALA:O	1:B:494:VAL:HG23	1.96	0.65
1:B:551:GLU:HA	1:B:551:GLU:OE2	1.97	0.65
1:B:673:HIS:HB3	1:B:675:GLU:OE2	1.96	0.65
1:A:470:ILE:O	1:A:471:GLN:HB2	1.96	0.65
1:A:559:GLU:HA	1:A:700:LEU:HB2	1.77	0.65
1:A:470:ILE:O	1:A:470:ILE:HD13	1.97	0.65
1:A:714:VAL:HG11	1:A:768:ILE:HG22	1.79	0.65
1:A:410:ASN:OD1	1:A:412:LYS:HB2	1.97	0.65
1:A:441:ILE:HD11	1:A:445:ARG:CZ	2.27	0.65
1:B:745:LYS:HZ3	1:B:746:GLU:HG2	1.58	0.65
1:A:380:ASN:HB2	1:A:384:GLN:NE2	2.12	0.64
1:B:669:LEU:HD11	1:B:727:ALA:HB2	1.79	0.64
1:B:685:GLN:HE22	1:B:689:GLN:HE21	1.43	0.64
1:A:661:ARG:CD	1:A:733:HIS:NE2	2.60	0.64
1:B:380:ASN:HB3	1:B:541:ASN:HD22	1.63	0.64
1:B:558:MET:HE2	1:B:653:LYS:HG2	1.80	0.64
1:B:694:LEU:HD13	1:B:763:ARG:NH2	2.07	0.64
1:A:547:ILE:O	1:A:551:GLU:HG3	1.97	0.64
1:A:782:ILE:HD13	1:A:783:PRO:O	1.97	0.64
1:A:696:ARG:NH2	1:B:408:THR:O	2.31	0.64
1:B:446:TYR:O	1:B:450:VAL:HG23	1.97	0.64
1:B:695:MET:CE	1:B:700:LEU:HD22	2.27	0.63
1:A:762:GLN:HA	1:A:762:GLN:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HA	1:B:388:ILE:HG12	1.81	0.63
1:A:381:THR:O	1:A:383:GLN:N	2.33	0.62
1:A:657:LEU:HD11	1:A:661:ARG:NH1	2.14	0.62
1:B:708:MET:HE2	1:B:719:LEU:HD21	1.81	0.62
1:A:746:GLU:C	1:A:748:GLU:H	2.02	0.62
1:B:411:PRO:O	1:B:415:ILE:HG23	1.99	0.62
1:B:492:GLU:OE2	1:B:549:HIS:HE1	1.82	0.62
1:A:445:ARG:HH21	1:A:498:TYR:HB3	1.65	0.62
1:B:385:LEU:CD1	1:B:388:ILE:HD11	2.20	0.61
1:B:557:ILE:HA	1:B:561:LEU:HB2	1.80	0.61
1:A:782:ILE:HD13	1:A:782:ILE:C	2.21	0.61
1:A:729:LYS:HZ1	1:A:736:GLN:NE2	1.98	0.61
1:A:424:TYR:HD2	1:B:425:ILE:HD12	1.66	0.61
1:B:386:MET:HG3	3:B:45:HOH:O	2.01	0.61
1:B:661:ARG:HE	1:B:733:HIS:CE1	2.19	0.61
1:A:718:ASP:OD1	1:A:719:LEU:N	2.33	0.61
1:A:415:ILE:HD13	1:A:454:TYR:HE1	1.66	0.60
1:A:465:GLU:O	1:A:469:SER:HA	2.01	0.60
1:A:425:ILE:CG2	1:A:429:LYS:HE2	2.32	0.60
1:B:698:ARG:NH2	3:B:35:HOH:O	2.33	0.60
1:B:676:LEU:HD11	1:B:717:ILE:HG13	1.83	0.60
1:B:745:LYS:HZ1	1:B:746:GLU:HG2	1.62	0.60
1:B:709:TYR:OH	2:E:418:ALA:HA	2.02	0.60
2:C:420:GLU:O	2:C:424:ASP:OD1	2.20	0.60
1:A:519:ASN:O	1:B:417:LYS:HE3	2.01	0.59
1:A:429:LYS:HE3	3:B:182:HOH:O	2.01	0.59
1:B:579:ARG:HG2	1:B:643:LYS:HD2	1.84	0.59
2:E:412:TYR:CD2	2:E:414:TRP:NE1	2.70	0.59
1:A:729:LYS:HZ1	1:A:736:GLN:HE21	1.44	0.59
1:A:559:GLU:OE2	1:A:661:ARG:NH1	2.35	0.59
1:A:733:HIS:N	1:A:733:HIS:ND1	2.51	0.59
1:A:668:ARG:HH11	1:A:668:ARG:CB	2.15	0.59
1:A:669:LEU:HD11	1:A:727:ALA:HB2	1.85	0.59
1:A:684:PHE:CZ	1:A:704:MET:HB2	2.39	0.58
1:A:685:GLN:HE22	1:A:689:GLN:HE22	1.50	0.58
1:B:491:LEU:O	1:B:495:MET:HG2	2.03	0.58
1:A:470:ILE:HD13	3:A:165:HOH:O	2.03	0.58
1:B:559:GLU:HB3	1:B:661:ARG:HH12	1.69	0.58
1:A:766:THR:HG22	3:A:95:HOH:O	2.02	0.58
1:A:569:LEU:HD22	1:A:573:ILE:HG13	1.85	0.58
1:B:578:THR:O	1:B:580:GLU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PRO:HD3	1:A:556:ARG:NH1	2.18	0.57
1:B:380:ASN:HB2	1:B:541:ASN:O	2.04	0.57
1:B:383:GLN:NE2	1:B:386:MET:SD	2.77	0.57
1:A:677:GLU:O	1:A:681:TRP:N	2.32	0.57
1:B:383:GLN:HA	1:B:383:GLN:NE2	2.17	0.57
1:B:766:THR:HG23	1:B:767:ASN:ND2	2.20	0.57
1:B:661:ARG:NE	1:B:733:HIS:CE1	2.73	0.57
1:B:418:ARG:HH11	1:B:480:ASN:HD22	1.52	0.57
1:A:559:GLU:HB2	1:A:661:ARG:HH22	1.70	0.56
1:A:678:HIS:CD2	1:A:779:LEU:HD23	2.40	0.56
1:B:400:LEU:HD22	1:B:404:PHE:CE1	2.40	0.56
1:B:418:ARG:O	1:B:422:ILE:HG12	2.05	0.56
1:B:467:ARG:HH22	1:B:468:LEU:HD11	1.69	0.56
1:A:558:MET:CE	1:A:653:LYS:HB3	2.34	0.56
1:B:579:ARG:CG	1:B:643:LYS:HD2	2.35	0.56
1:B:669:LEU:HD23	1:B:719:LEU:HD11	1.87	0.56
1:B:434:VAL:HG11	1:B:510:THR:N	2.19	0.56
1:A:656:ARG:NH2	1:A:784:HIS:HA	2.20	0.56
1:B:785:ILE:HG13	1:B:785:ILE:OXT	2.06	0.56
1:B:418:ARG:HA	3:B:183:HOH:O	2.05	0.56
1:A:512:LEU:HB2	1:A:516:TRP:CG	2.40	0.56
1:B:411:PRO:HB3	1:B:478:ASN:ND2	2.21	0.56
1:B:668:ARG:HD3	1:B:730:ASP:OD2	2.06	0.55
1:A:657:LEU:HD11	1:A:661:ARG:CZ	2.36	0.55
1:A:445:ARG:NH2	1:A:498:TYR:HB3	2.22	0.55
1:A:685:GLN:NE2	1:A:689:GLN:NE2	2.50	0.55
1:A:434:VAL:HG13	1:A:505:ASN:O	2.07	0.55
1:A:701:ASP:OD2	1:A:733:HIS:HD2	1.90	0.55
1:B:669:LEU:HD11	1:B:727:ALA:CB	2.36	0.55
1:B:656:ARG:CZ	1:B:785:ILE:HG23	2.37	0.55
1:B:663:ASN:HA	1:B:677:GLU:OE2	2.07	0.55
1:B:745:LYS:NZ	1:B:746:GLU:CG	2.65	0.55
1:A:661:ARG:HD3	1:A:733:HIS:NE2	2.22	0.54
2:E:419:GLY:O	2:E:420:GLU:HB2	2.07	0.54
1:A:487:LEU:HD22	1:A:491:LEU:CD1	2.36	0.54
1:A:669:LEU:N	1:A:669:LEU:HD12	2.22	0.54
1:B:714:VAL:HB	1:B:772:ALA:HB2	1.89	0.54
2:E:412:TYR:CD2	2:E:414:TRP:CD1	2.94	0.54
1:A:520:VAL:HG12	1:A:521:LEU:HD12	1.89	0.54
1:A:656:ARG:HH21	1:A:784:HIS:HA	1.73	0.54
1:B:543:THR:HB	1:B:545:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:O	1:A:381:THR:O	2.25	0.54
1:A:782:ILE:HG23	1:A:784:HIS:NE2	2.23	0.54
1:B:736:GLN:HA	1:B:739:PHE:CE2	2.43	0.54
1:B:514:PHE:HB3	1:B:515:PRO:HD3	1.90	0.54
2:D:420:GLU:O	2:D:421:GLY:O	2.26	0.54
1:B:691:GLU:HB3	1:B:694:LEU:HD23	1.89	0.53
1:A:729:LYS:NZ	1:A:736:GLN:NE2	2.47	0.53
1:B:733:HIS:ND1	1:B:733:HIS:N	2.54	0.53
1:A:386:MET:HG2	3:A:239:HOH:O	2.08	0.53
1:B:720:LYS:N	1:B:720:LYS:HD3	2.23	0.53
1:A:411:PRO:O	1:A:415:ILE:HG23	2.08	0.53
1:B:658:ALA:HB1	1:B:684:PHE:CE2	2.44	0.53
1:B:661:ARG:HG2	1:B:733:HIS:CE1	2.44	0.53
1:A:543:THR:HB	1:A:545:GLU:OE2	2.09	0.53
1:B:661:ARG:NE	1:B:733:HIS:NE2	2.57	0.53
1:A:456:VAL:HG12	1:A:460:MET:CE	2.40	0.52
1:B:380:ASN:CG	1:B:541:ASN:HA	2.28	0.52
1:B:493:VAL:HG13	1:B:546:MET:HG2	1.90	0.52
1:A:380:ASN:O	1:A:381:THR:C	2.47	0.52
1:B:745:LYS:CE	1:B:746:GLU:HG2	2.39	0.52
1:A:661:ARG:NE	1:A:733:HIS:CE1	2.77	0.52
1:A:407:CYS:SG	1:A:477:LEU:HD12	2.49	0.52
1:A:515:PRO:HD2	3:A:169:HOH:O	2.08	0.52
1:B:382:ILE:HG23	1:B:383:GLN:HG2	1.91	0.52
1:A:417:LYS:NZ	1:A:417:LYS:HB3	2.25	0.52
1:A:493:VAL:HA	1:A:546:MET:HE1	1.91	0.51
1:A:502:THR:O	1:A:504:GLN:O	2.27	0.51
1:A:575:GLN:HG2	1:A:579:ARG:CD	2.40	0.51
1:A:661:ARG:HG2	1:A:733:HIS:CE1	2.44	0.51
1:B:453:TYR:CE1	1:B:486:LEU:HD23	2.45	0.51
1:B:665:LEU:HD23	1:B:731:LEU:HD11	1.93	0.51
1:B:684:PHE:CE2	1:B:704:MET:HB2	2.45	0.51
1:A:761:MET:O	1:A:765:LYS:N	2.44	0.51
1:B:410:ASN:OD1	1:B:412:LYS:HB2	2.10	0.51
1:B:775:ARG:NH1	2:E:410:ASP:OD2	2.42	0.51
1:A:669:LEU:HD21	1:A:724:ILE:HA	1.92	0.51
1:A:685:GLN:OE1	1:A:686:HIS:HD2	1.92	0.51
1:A:745:LYS:HG3	1:A:746:GLU:OE2	2.10	0.51
1:B:380:ASN:HA	1:B:384:GLN:HG2	1.93	0.51
1:B:432:LYS:HD3	1:B:432:LYS:N	2.26	0.51
1:B:529:TYR:CE2	1:B:530:LYS:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:MET:HG2	3:B:244:HOH:O	2.11	0.51
1:A:767:ASN:ND2	3:A:243:HOH:O	2.43	0.51
1:B:395:GLN:HG3	3:B:231:HOH:O	2.10	0.51
1:B:385:LEU:HD22	1:B:385:LEU:N	2.27	0.50
1:B:689:GLN:HG2	1:B:690:ASN:ND2	2.26	0.50
1:B:695:MET:HE2	1:B:700:LEU:HD22	1.93	0.50
1:B:756:TYR:HA	1:B:760:PHE:HB3	1.92	0.50
1:A:493:VAL:HA	1:A:546:MET:CE	2.42	0.50
1:A:575:GLN:CG	1:A:579:ARG:HD2	2.41	0.50
1:A:698:ARG:HG2	3:A:82:HOH:O	2.10	0.50
1:A:774:THR:CG2	1:A:775:ARG:HD3	2.24	0.50
1:A:655:TYR:OH	1:A:689:GLN:HB2	2.11	0.50
1:A:709:TYR:OH	1:A:713:LYS:NZ	2.45	0.50
1:B:390:ASN:HA	1:B:451:ARG:NH1	2.26	0.50
2:E:413:LEU:CD1	2:E:413:LEU:N	2.74	0.50
1:A:434:VAL:HG12	1:A:434:VAL:O	2.11	0.50
1:B:684:PHE:CZ	1:B:704:MET:HB2	2.46	0.50
1:A:528:PHE:CE2	1:A:532:ILE:HD11	2.46	0.50
2:D:422:ILE:HD11	2:D:426:PHE:CE1	2.45	0.50
1:B:578:THR:O	1:B:580:GLU:HG3	2.10	0.50
1:A:507:ASP:HA	3:A:139:HOH:O	2.12	0.50
1:B:514:PHE:CD1	1:B:514:PHE:C	2.85	0.50
1:B:533:GLU:HB2	2:D:412:TYR:OH	2.12	0.50
1:B:576:SER:C	1:B:578:THR:H	2.15	0.50
1:B:766:THR:HG23	1:B:767:ASN:N	2.27	0.50
1:A:382:ILE:HD12	1:A:382:ILE:O	2.12	0.49
1:B:520:VAL:HG12	1:B:521:LEU:HD12	1.94	0.49
2:C:420:GLU:O	2:C:421:GLY:O	2.30	0.49
2:D:420:GLU:HA	2:D:424:ASP:OD1	2.12	0.49
1:A:581:GLY:O	1:A:643:LYS:HB3	2.12	0.49
1:B:558:MET:HE1	1:B:653:LYS:HB3	1.94	0.49
1:B:668:ARG:HD2	3:B:173:HOH:O	2.13	0.49
1:A:472:ASN:O	1:A:473:PHE:HB2	2.13	0.49
1:A:682:THR:HA	1:A:780:SER:OG	2.12	0.49
1:A:685:GLN:NE2	1:A:689:GLN:HE21	2.11	0.49
1:B:484:MET:HA	1:B:484:MET:CE	2.41	0.49
2:C:417:GLU:N	2:C:420:GLU:OE2	2.41	0.49
1:A:731:LEU:HD13	1:A:733:HIS:NE2	2.28	0.49
1:B:385:LEU:N	1:B:385:LEU:CD2	2.75	0.49
1:B:464:GLU:OE1	1:B:467:ARG:NH2	2.45	0.49
1:B:722:LYS:HG3	1:B:723:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:GLY:HA3	1:B:491:LEU:HD23	1.94	0.49
1:A:383:GLN:HG3	3:A:26:HOH:O	2.13	0.49
1:A:520:VAL:HG12	1:A:521:LEU:CD1	2.43	0.49
1:B:380:ASN:CB	1:B:541:ASN:HD22	2.26	0.49
1:B:384:GLN:O	1:B:387:MET:HB3	2.12	0.49
1:B:669:LEU:HD21	1:B:724:ILE:HA	1.94	0.48
1:B:725:VAL:HG13	1:B:739:PHE:CZ	2.48	0.48
1:B:729:LYS:NZ	1:B:729:LYS:HB3	2.28	0.48
1:A:689:GLN:HG2	1:A:690:ASN:HD21	1.76	0.48
2:E:412:TYR:HE2	2:E:414:TRP:NE1	2.05	0.48
1:B:528:PHE:O	1:B:531:VAL:HG12	2.13	0.48
1:A:429:LYS:HE3	1:A:520:VAL:O	2.13	0.48
1:A:661:ARG:NE	1:A:733:HIS:NE2	2.62	0.48
1:B:772:ALA:HB1	2:E:412:TYR:CD2	2.49	0.48
1:A:559:GLU:HG3	1:A:699:HIS:NE2	2.28	0.48
1:B:569:LEU:O	1:B:573:ILE:HG13	2.13	0.48
1:B:720:LYS:O	1:B:723:ILE:HB	2.14	0.48
1:A:395:GLN:OE1	1:A:395:GLN:HA	2.14	0.47
1:A:386:MET:CE	1:A:448:LEU:HD13	2.43	0.47
1:A:782:ILE:HD12	1:A:784:HIS:CD2	2.49	0.47
1:B:433:ALA:O	1:B:434:VAL:HB	2.13	0.47
1:A:497:THR:HG22	1:A:546:MET:SD	2.54	0.47
1:A:512:LEU:O	1:A:513:SER:O	2.30	0.47
1:B:729:LYS:CE	1:B:736:GLN:HG3	2.42	0.47
1:A:460:MET:HE1	1:A:486:LEU:CD2	2.34	0.47
1:B:417:LYS:NZ	3:B:182:HOH:O	2.41	0.47
1:A:408:THR:HB	1:B:571:ASP:OD1	2.14	0.47
1:A:438:CYS:O	1:A:441:ILE:CG2	2.59	0.47
1:A:386:MET:HE3	1:A:448:LEU:HD13	1.97	0.47
1:A:400:LEU:HD22	1:A:457:MET:HE3	1.97	0.47
1:A:746:GLU:C	1:A:748:GLU:N	2.67	0.47
1:A:757:ASN:O	1:A:762:GLN:HG2	2.15	0.47
1:A:578:THR:HG22	1:A:579:ARG:N	2.29	0.47
1:A:746:GLU:O	1:A:748:GLU:N	2.46	0.47
1:B:554:GLU:OE1	1:B:653:LYS:HD3	2.14	0.47
1:B:404:PHE:O	1:B:407:CYS:HB2	2.14	0.47
2:C:421:GLY:HA2	3:C:106:HOH:O	2.15	0.47
1:A:467:ARG:NH2	2:C:424:ASP:OD1	2.48	0.46
1:A:659:TYR:CZ	1:A:782:ILE:HG13	2.51	0.46
1:B:523:LEU:HD13	1:B:528:PHE:HB2	1.97	0.46
1:A:675:GLU:H	1:A:675:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:GLU:HG2	2:D:423:SER:OG	2.15	0.46
1:A:694:LEU:HA	1:A:698:ARG:HH21	1.80	0.46
1:B:656:ARG:HB2	2:D:413:LEU:HD22	1.97	0.46
1:B:725:VAL:HG13	1:B:739:PHE:CE2	2.50	0.46
1:B:691:GLU:O	1:B:694:LEU:HB2	2.15	0.46
1:A:504:GLN:O	1:A:505:ASN:OD1	2.34	0.46
1:B:656:ARG:HG2	2:D:413:LEU:CB	2.40	0.46
1:B:745:LYS:HZ3	1:B:746:GLU:CG	2.26	0.46
1:A:559:GLU:CB	1:A:661:ARG:HH22	2.29	0.46
1:B:385:LEU:C	1:B:387:MET:N	2.68	0.46
1:B:656:ARG:NH2	1:B:785:ILE:OXT	2.49	0.46
1:B:438:CYS:HB2	1:B:441:ILE:CD1	2.44	0.46
1:A:385:LEU:HG	1:A:539:GLU:OE1	2.16	0.46
1:A:756:TYR:HA	1:A:760:PHE:HB3	1.97	0.45
1:A:782:ILE:HG23	1:A:784:HIS:CE1	2.51	0.45
1:B:401:ILE:HG22	1:B:405:ASN:HD21	1.81	0.45
1:B:536:ILE:HG12	1:B:550:LEU:HD12	1.99	0.45
1:A:408:THR:H	1:A:474:SER:HB2	1.80	0.45
1:A:456:VAL:HG12	1:A:460:MET:HE1	1.98	0.45
1:A:665:LEU:HD21	1:A:728:TYR:HA	1.97	0.45
1:A:650:PHE:O	1:A:654:VAL:HG23	2.17	0.45
1:B:415:ILE:CD1	1:B:454:TYR:HE1	2.30	0.45
1:B:554:GLU:OE2	2:D:412:TYR:CE1	2.69	0.45
1:B:576:SER:C	1:B:578:THR:N	2.70	0.45
1:B:661:ARG:CD	1:B:733:HIS:NE2	2.80	0.45
1:B:727:ALA:HB1	3:B:173:HOH:O	2.15	0.45
1:A:422:ILE:HD11	1:A:484:MET:CE	2.47	0.45
1:B:401:ILE:HG22	1:B:405:ASN:ND2	2.31	0.45
1:B:662:LEU:HD21	1:B:680:ILE:HG21	1.99	0.45
1:A:514:PHE:CD1	1:A:514:PHE:C	2.88	0.45
1:B:382:ILE:O	1:B:386:MET:HG3	2.17	0.45
1:B:444:GLN:O	1:B:444:GLN:OE1	2.34	0.45
1:B:692:TYR:O	1:B:695:MET:HB2	2.17	0.45
1:A:418:ARG:HB3	3:A:116:HOH:O	2.16	0.45
1:B:467:ARG:NH2	1:B:468:LEU:HG	2.31	0.45
1:B:485:SER:HA	1:B:523:LEU:HD11	2.00	0.45
1:A:669:LEU:N	1:A:669:LEU:CD1	2.78	0.44
1:B:533:GLU:OE2	2:D:416:LEU:HB2	2.18	0.44
1:A:693:GLU:OE2	1:A:696:ARG:NH1	2.48	0.44
1:B:784:HIS:O	1:B:785:ILE:CG2	2.65	0.44
1:A:482:PHE:HA	2:C:426:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:PHE:O	1:B:529:TYR:HD2	2.01	0.44
1:A:514:PHE:N	3:A:169:HOH:O	2.51	0.44
1:A:762:GLN:HE21	1:A:762:GLN:CA	2.22	0.44
1:A:514:PHE:O	1:A:516:TRP:N	2.50	0.44
1:A:661:ARG:HG2	1:A:733:HIS:NE2	2.33	0.44
1:B:548:LYS:HE2	1:B:548:LYS:HA	2.00	0.44
1:A:656:ARG:HH21	1:A:784:HIS:CA	2.30	0.44
1:B:708:MET:CE	1:B:719:LEU:HD21	2.46	0.44
1:B:715:LYS:NZ	3:B:137:HOH:O	2.50	0.44
2:E:410:ASP:N	2:E:410:ASP:OD2	2.50	0.43
1:A:475:LYS:HA	1:A:475:LYS:HD2	1.83	0.43
1:A:679:ILE:HD13	1:A:715:LYS:HE3	2.00	0.43
1:B:691:GLU:HB3	1:B:694:LEU:CD2	2.48	0.43
1:A:770:GLN:O	1:A:777:PRO:HD3	2.18	0.43
1:B:467:ARG:NH1	2:D:420:GLU:O	2.50	0.43
1:B:656:ARG:HG2	2:D:413:LEU:HD22	2.00	0.43
1:B:716:ASN:HA	2:E:414:TRP:CH2	2.53	0.43
1:A:691:GLU:O	1:A:694:LEU:HB2	2.18	0.43
1:B:500:ARG:NH2	3:B:102:HOH:O	2.50	0.43
1:B:525:ALA:HB1	1:B:557:ILE:HG12	2.00	0.43
1:A:384:GLN:HB2	1:A:384:GLN:HE21	1.66	0.43
1:A:441:ILE:HD11	1:A:445:ARG:NH2	2.33	0.43
1:A:504:GLN:O	1:A:505:ASN:C	2.54	0.43
1:A:521:LEU:O	1:A:522:ASN:C	2.57	0.43
1:A:556:ARG:NH2	3:A:56:HOH:O	2.48	0.43
1:B:493:VAL:HG13	1:B:546:MET:CG	2.49	0.43
1:B:576:SER:O	1:B:578:THR:N	2.51	0.43
1:A:539:GLU:HG3	1:A:542:LEU:HG	2.00	0.43
1:B:682:THR:HA	1:B:780:SER:OG	2.19	0.43
1:A:579:ARG:O	1:A:579:ARG:HD3	2.18	0.43
1:A:691:GLU:HG3	1:A:764:LEU:CD2	2.42	0.43
1:B:484:MET:HA	1:B:484:MET:HE2	2.00	0.43
1:A:691:GLU:HB3	1:A:694:LEU:HD22	2.01	0.43
1:B:685:GLN:NE2	1:B:689:GLN:HE21	2.12	0.43
1:B:729:LYS:HA	1:B:734:ALA:HB1	1.99	0.43
1:A:507:ASP:O	1:A:508:SER:HB2	2.18	0.42
1:A:381:THR:C	1:A:383:GLN:H	2.23	0.42
1:A:385:LEU:CD2	1:A:389:LEU:HG	2.47	0.42
1:A:421:ASP:HA	1:A:424:TYR:CD2	2.54	0.42
1:B:423:GLY:HA2	1:B:446:TYR:CE2	2.54	0.42
1:A:380:ASN:O	1:A:380:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLU:OE1	1:A:541:ASN:HB2	2.19	0.42
1:A:725:VAL:HG22	1:A:739:PHE:CG	2.54	0.42
1:B:387:MET:SD	1:B:388:ILE:N	2.92	0.42
1:B:558:MET:HE1	1:B:654:VAL:N	2.33	0.42
1:A:580:GLU:H	1:A:580:GLU:HG2	1.62	0.42
1:A:381:THR:C	1:A:383:GLN:N	2.72	0.42
1:A:656:ARG:HD2	3:A:73:HOH:O	2.19	0.42
1:B:545:GLU:CD	1:B:545:GLU:H	2.23	0.42
1:A:465:GLU:O	1:A:469:SER:N	2.52	0.42
1:A:552:ARG:O	1:A:556:ARG:HG3	2.20	0.42
1:B:432:LYS:HD3	1:B:432:LYS:H	1.83	0.42
1:B:713:LYS:HE3	2:E:415:GLY:O	2.19	0.42
1:A:425:ILE:HG13	1:B:425:ILE:HD11	2.02	0.42
1:A:687:THR:O	1:A:691:GLU:HB2	2.20	0.42
1:B:400:LEU:HD22	1:B:404:PHE:CZ	2.54	0.42
1:B:556:ARG:O	1:B:559:GLU:HG2	2.20	0.42
1:B:720:LYS:N	1:B:720:LYS:CD	2.83	0.42
1:A:383:GLN:HA	3:A:26:HOH:O	2.19	0.42
1:A:384:GLN:O	1:A:387:MET:HB3	2.18	0.42
1:A:714:VAL:CG1	1:A:768:ILE:HG22	2.46	0.42
1:A:720:LYS:HD2	1:A:722:LYS:HE2	2.02	0.42
1:B:412:LYS:O	1:B:416:LEU:HG	2.20	0.42
1:A:436:ALA:HA	1:A:439:VAL:HG13	2.02	0.41
1:A:687:THR:HG23	1:A:691:GLU:HB2	2.02	0.41
1:A:745:LYS:C	1:A:746:GLU:O	2.59	0.41
1:A:424:TYR:CD2	1:B:425:ILE:HD12	2.50	0.41
1:A:552:ARG:HD2	1:A:552:ARG:HA	1.65	0.41
1:B:456:VAL:O	1:B:460:MET:HB2	2.19	0.41
1:A:430:PHE:CE2	1:A:495:MET:HE1	2.55	0.41
1:A:436:ALA:O	1:A:439:VAL:HG13	2.21	0.41
1:B:701:ASP:OD2	1:B:733:HIS:CD2	2.62	0.41
1:A:776:PRO:HA	1:A:777:PRO:HD3	1.91	0.41
1:A:729:LYS:NZ	1:A:736:GLN:HG2	2.36	0.41
1:B:388:ILE:HG13	1:B:389:LEU:N	2.36	0.41
1:B:698:ARG:NH1	1:B:743:LEU:O	2.49	0.41
1:B:695:MET:HE1	1:B:700:LEU:HD22	2.02	0.41
1:A:461:LEU:HD11	1:A:477:LEU:HD21	2.02	0.41
1:A:526:PHE:O	1:A:529:TYR:HD2	2.04	0.41
1:A:548:LYS:HD2	1:A:548:LYS:HA	1.84	0.41
1:B:433:ALA:O	1:B:434:VAL:CB	2.68	0.41
1:A:434:VAL:HG12	1:A:438:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:LEU:O	1:A:669:LEU:HD13	2.20	0.41
1:A:465:GLU:O	1:A:469:SER:CA	2.69	0.40
1:A:513:SER:HB3	3:A:169:HOH:O	2.20	0.40
1:A:514:PHE:C	1:A:516:TRP:N	2.74	0.40
1:B:708:MET:HE2	1:B:708:MET:HB3	2.01	0.40
1:B:645:THR:HG21	2:D:424:ASP:O	2.21	0.40
1:A:782:ILE:HD12	1:A:784:HIS:NE2	2.37	0.40
1:B:383:GLN:NE2	1:B:383:GLN:CA	2.77	0.40
1:B:498:TYR:C	1:B:500:ARG:H	2.24	0.40
1:A:657:LEU:HD21	1:A:661:ARG:HE	1.86	0.40
1:B:381:THR:HA	1:B:543:THR:HG22	2.03	0.40
1:B:387:MET:HE1	1:B:388:ILE:HA	2.04	0.40
2:C:410:ASP:N	3:C:250:HOH:O	2.54	0.40
1:A:409:VAL:O	1:A:411:PRO:HD3	2.22	0.40
1:A:750:ASP:CG	1:A:754:VAL:HG21	2.41	0.40
1:B:479:ASP:OD1	2:D:426:PHE:HB3	2.21	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	343/345 (99%)	303 (88%)	23 (7%)	17 (5%)	2 0
1	B	334/345 (97%)	301 (90%)	23 (7%)	10 (3%)	4 2
2	C	16/18 (89%)	15 (94%)	0	1 (6%)	1 0
2	D	16/18 (89%)	11 (69%)	3 (19%)	2 (12%)	0 0
2	E	10/18 (56%)	5 (50%)	2 (20%)	3 (30%)	0 0
All	All	719/744 (97%)	635 (88%)	51 (7%)	33 (5%)	2 1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	THR
1	A	382	ILE
1	A	507	ASP
1	A	513	SER
1	A	718	ASP
1	A	734	ALA
1	B	433	ALA
1	B	579	ARG
1	B	784	HIS
2	C	421	GLY
2	E	411	ASP
2	E	412	TYR
1	B	434	VAL
1	B	513	SER
2	D	421	GLY
1	A	469	SER
1	A	472	ASN
1	A	508	SER
1	B	435	GLY
1	B	439	VAL
2	D	417	GLU
2	E	420	GLU
1	A	512	LEU
1	A	580	GLU
1	A	644	SER
1	A	676	LEU
1	A	746	GLU
1	A	560	SER
1	A	719	LEU
1	B	577	LYS
1	B	746	GLU
1	A	747	GLU
1	B	388	ILE

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	321/321 (100%)	287 (89%)	34 (11%)	6 6
1	B	315/321 (98%)	296 (94%)	19 (6%)	19 22
2	C	14/14 (100%)	14 (100%)	0	100 100
2	D	14/14 (100%)	14 (100%)	0	100 100
2	E	8/14 (57%)	4 (50%)	4 (50%)	0 0
All	All	672/684 (98%)	615 (92%)	57 (8%)	10 10

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	381	THR
1	A	382	ILE
1	A	383	GLN
1	A	384	GLN
1	A	385	LEU
1	A	398	GLU
1	A	412	LYS
1	A	445	ARG
1	A	464	GLU
1	A	470	ILE
1	A	484	MET
1	A	486	LEU
1	A	487	LEU
1	A	495	MET
1	A	511	ASP
1	A	521	LEU
1	A	529	TYR
1	A	531	VAL
1	A	558	MET
1	A	569	LEU
1	A	579	ARG
1	A	657	LEU
1	A	662	LEU
1	A	678	HIS
1	A	683	LEU
1	A	694	LEU
1	A	700	LEU
1	A	721	PHE
1	A	725	VAL
1	A	733	HIS

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Mol	Chain	Res	Type
1	A	758	SER
1	A	775	ARG
1	A	782	ILE
1	B	383	GLN
1	B	387	MET
1	B	395	GLN
1	B	400	LEU
1	B	415	ILE
1	B	432	LYS
1	B	452	LEU
1	B	514	PHE
1	B	523	LEU
1	B	529	TYR
1	B	548	LYS
1	B	569	LEU
1	B	683	LEU
1	B	694	LEU
1	B	700	LEU
1	B	713	LYS
1	B	732	PRO
1	B	733	HIS
1	B	778	THR
2	E	410	ASP
2	E	411	ASP
2	E	412	TYR
2	E	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	384	GLN
1	A	390	ASN
1	A	406	ASN
1	A	541	ASN
1	A	678	HIS
1	A	686	HIS
1	A	689	GLN
1	A	690	ASN
1	A	736	GLN
1	A	762	GLN
1	A	767	ASN

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Mol	Chain	Res	Type
1	B	380	ASN
1	B	383	GLN
1	B	395	GLN
1	B	444	GLN
1	B	478	ASN
1	B	480	ASN
1	B	541	ASN
1	B	549	HIS
1	B	678	HIS
1	B	689	GLN
1	B	690	ASN
1	B	733	HIS
1	B	736	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.