Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:13 PM GMT

PDB ID	:	1SNX
Title	:	CRYSTAL STRUCTURE OF APO INTERLEUKIN-2 TYROSINE KINASE CATALYTIC DOMAIN
Authors	:	Brown, K.; Long, J.M.; Vial, S.C.; Dedi, N.; Dunster, N.J.; Renwick, S.B.; Tanner, A.J.; Frantz, J.D.; Fleming, M.A.; Cheetham, G.M.T.
Deposited on	:	2004-03-12
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

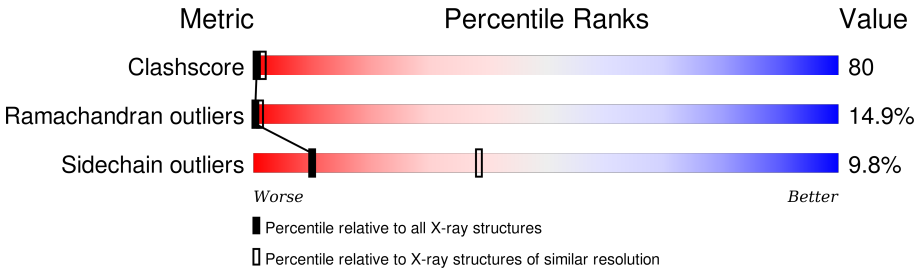
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	17% 62% 13% • 7%
1	B	264	20% 54% 17% • 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3912 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 Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1956	1249	326	365	16			
1	B	245	Total	C	N	O	S	0	0	0
			1956	1249	326	365	16			

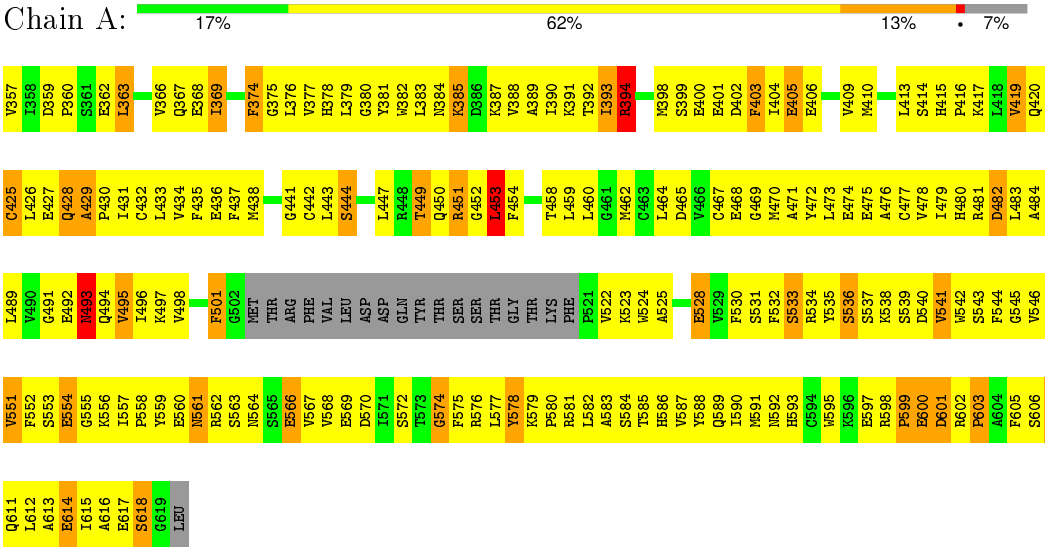
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

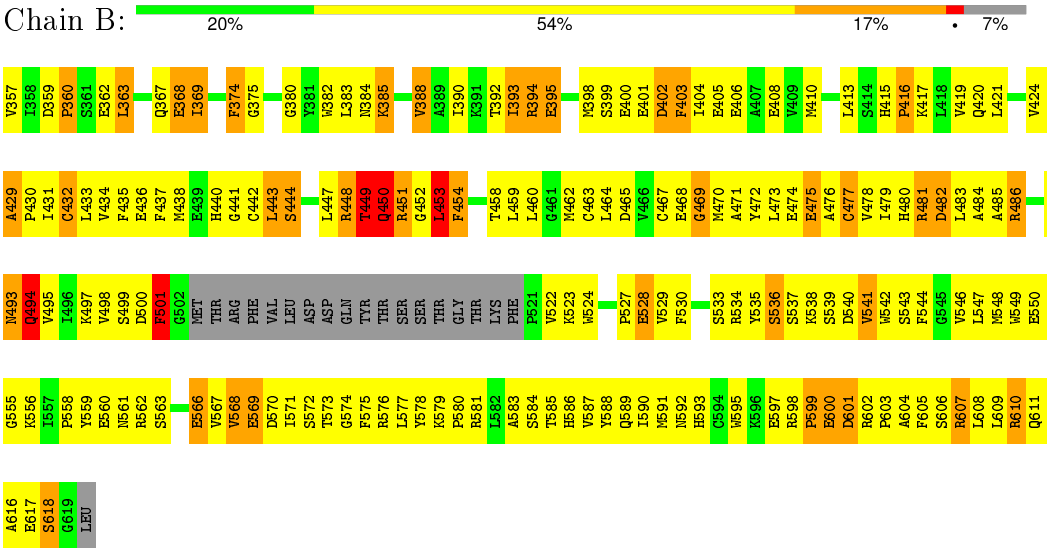
- Molecule 1: Tyrosine-protein kinase ITK/TSK

Chain A:



- Molecule 1: Tyrosine-protein kinase ITK/TSK

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	39.50Å 54.90Å 59.20Å 92.50° 85.50° 74.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	49.0 (20.00-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.241 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3912	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.52	0/2000	0.78	0/2700
1	B	0.52	0/2000	0.78	1/2700 (0.0%)
All	All	0.52	0/4000	0.78	1/5400 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	491	GLY	N-CA-C	5.50	126.84	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1956	0	1913	304	1
1	B	1956	0	1913	312	1
All	All	3912	0	3826	616	1

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 80.

All (616) 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:459:LEU:HA	1:B:462:MET:HE3	1.25	1.14
1:B:580:PRO:HG2	1:B:583:ALA:HB2	1.16	1.13
1:B:375:GLY:HA2	1:B:392:THR:O	1.51	1.09
1:B:392:THR:HA	1:B:432:CYS:HB3	1.28	1.08
1:B:360:PRO:HG2	1:B:362:GLU:HG3	1.34	1.07
1:B:607:ARG:HH11	1:B:607:ARG:HB2	1.24	1.02
1:A:607:ARG:HB2	1:A:607:ARG:HH11	1.26	0.99
1:A:359:ASP:OD2	1:A:423:GLY:HA3	1.63	0.98
1:B:450:GLN:O	1:B:453:LEU:HG	1.63	0.97
1:A:390:ILE:HG23	1:A:434:VAL:HG22	1.49	0.94
1:A:398:MET:HE3	1:A:403:PHE:HB2	1.50	0.93
1:B:611:GLN:O	1:B:614:GLU:HB2	1.70	0.92
1:B:607:ARG:O	1:B:611:GLN:HG3	1.68	0.91
1:A:464:LEU:HD21	1:A:612:LEU:HB2	1.48	0.91
1:B:429:ALA:HB1	1:B:430:PRO:HD2	1.52	0.91
1:B:501:PHE:H	1:B:501:PHE:HD2	1.18	0.91
1:A:501:PHE:HD2	1:A:501:PHE:H	1.19	0.91
1:A:401:GLU:HG3	1:A:402:ASP:N	1.84	0.89
1:B:475:GLU:C	1:B:477:CYS:H	1.71	0.89
1:A:398:MET:CE	1:A:403:PHE:HB2	2.02	0.89
1:B:600:GLU:HG2	1:B:601:ASP:OD1	1.71	0.89
1:A:360:PRO:HG2	1:A:362:GLU:HG3	1.55	0.87
1:B:610:ARG:O	1:B:613:ALA:HB3	1.73	0.87
1:A:399:SER:HB2	1:A:402:ASP:HB2	1.55	0.87
1:A:580:PRO:HG2	1:A:583:ALA:HB2	1.54	0.86
1:B:585:THR:O	1:B:589:GLN:HG3	1.75	0.85
1:A:450:GLN:O	1:A:453:LEU:HG	1.78	0.83
1:A:392:THR:HA	1:A:432:CYS:HB3	1.60	0.83
1:A:401:GLU:HG3	1:A:402:ASP:H	1.40	0.82
1:B:464:LEU:HD21	1:B:612:LEU:HB2	1.61	0.82
1:B:421:LEU:HA	1:B:435:PHE:HA	1.61	0.82
1:B:607:ARG:NH1	1:B:607:ARG:HB2	1.94	0.81
1:B:399:SER:HB2	1:B:402:ASP:HB2	1.63	0.81
1:A:542:TRP:HH2	1:A:576:ARG:HH21	1.28	0.80
1:B:459:LEU:CA	1:B:462:MET:HE3	2.11	0.80
1:B:360:PRO:HG2	1:B:362:GLU:CG	2.12	0.79
1:B:473:LEU:HB3	1:B:478:VAL:HB	1.65	0.79
1:A:617:GLU:O	1:A:618:SER:HB2	1.82	0.78
1:A:542:TRP:HH2	1:A:576:ARG:NH2	1.81	0.78
1:B:599:PRO:O	1:B:602:ARG:N	2.11	0.78
1:A:605:PHE:HA	1:A:608:LEU:HD12	1.66	0.78
1:A:475:GLU:C	1:A:477:CYS:H	1.88	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLU:O	1:B:404:ILE:HG13	1.85	0.76
1:B:549:TRP:CZ3	1:B:556:LYS:O	2.38	0.76
1:A:442:CYS:HA	1:A:489:LEU:HD23	1.67	0.76
1:A:424:VAL:HG13	1:A:433:LEU:HD12	1.68	0.76
1:B:375:GLY:CA	1:B:392:THR:O	2.33	0.76
1:B:392:THR:CA	1:B:432:CYS:HB3	2.12	0.76
1:A:433:LEU:HD23	1:A:435:PHE:CZ	2.21	0.76
1:B:383:LEU:O	1:B:384:ASN:HB3	1.86	0.75
1:A:482:ASP:O	1:A:487:ASN:ND2	2.20	0.75
1:A:600:GLU:HG2	1:A:601:ASP:OD1	1.86	0.74
1:A:534:ARG:O	1:A:534:ARG:HG2	1.84	0.74
1:A:532:PHE:O	1:A:533:SER:HB2	1.86	0.74
1:B:475:GLU:C	1:B:477:CYS:N	2.35	0.74
1:A:375:GLY:HA2	1:A:392:THR:O	1.88	0.74
1:B:540:ASP:O	1:B:543:SER:N	2.21	0.74
1:A:473:LEU:HA	1:A:476:ALA:HB3	1.69	0.74
1:B:552:PHE:C	1:B:554:GLU:H	1.90	0.73
1:A:591:MET:HB3	1:A:595:TRP:CH2	2.23	0.73
1:A:421:LEU:HD13	1:A:435:PHE:CD2	2.23	0.73
1:A:417:LYS:O	1:A:497:LYS:HA	1.88	0.73
1:A:464:LEU:HD22	1:A:609:LEU:HD12	1.69	0.73
1:B:580:PRO:CG	1:B:583:ALA:HB2	2.09	0.73
1:B:424:VAL:HG13	1:B:433:LEU:HD12	1.70	0.73
1:B:385:LYS:HD3	1:B:385:LYS:O	1.88	0.73
1:A:429:ALA:HB1	1:A:430:PRO:HD2	1.69	0.72
1:B:448:ARG:O	1:B:451:ARG:HB2	1.90	0.72
1:B:450:GLN:O	1:B:454:PHE:HE1	1.72	0.72
1:B:598:ARG:HB2	1:B:601:ASP:OD2	1.90	0.72
1:A:458:THR:HG22	1:A:462:MET:HE2	1.70	0.72
1:B:534:ARG:HG2	1:B:534:ARG:O	1.89	0.72
1:A:429:ALA:HB1	1:A:430:PRO:CD	2.19	0.71
1:B:393:ILE:HG12	1:B:431:ILE:O	1.89	0.71
1:B:417:LYS:C	1:B:497:LYS:HG2	2.11	0.71
1:A:561:ASN:O	1:A:562:ARG:HG3	1.91	0.70
1:A:613:ALA:O	1:A:617:GLU:HG3	1.92	0.70
1:A:422:TYR:HE1	1:A:436:GLU:HA	1.55	0.70
1:B:501:PHE:N	1:B:501:PHE:HD2	1.89	0.70
1:B:607:ARG:O	1:B:610:ARG:HB2	1.91	0.70
1:B:480:HIS:CD2	1:B:501:PHE:HB3	2.27	0.70
1:B:464:LEU:HD21	1:B:612:LEU:CB	2.20	0.70
1:B:570:ASP:O	1:B:575:PHE:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ALA:O	1:A:478:VAL:HG23	1.91	0.70
1:B:464:LEU:HD22	1:B:609:LEU:HD12	1.74	0.70
1:A:415:HIS:O	1:A:417:LYS:N	2.24	0.70
1:B:380:GLY:O	1:B:388:VAL:HG22	1.91	0.70
1:B:468:GLU:HG3	1:B:609:LEU:HD11	1.74	0.69
1:B:401:GLU:HA	1:B:404:ILE:HD12	1.72	0.69
1:A:452:GLY:O	1:A:454:PHE:N	2.25	0.69
1:A:523:LYS:HE2	1:A:559:TYR:HB2	1.75	0.69
1:A:393:ILE:HG12	1:A:431:ILE:O	1.93	0.69
1:B:419:VAL:HG21	1:B:499:SER:HB3	1.74	0.69
1:B:590:ILE:O	1:B:593:HIS:N	2.24	0.69
1:B:368:GLU:O	1:B:369:ILE:HG23	1.93	0.69
1:A:399:SER:HB2	1:A:402:ASP:CB	2.23	0.69
1:B:429:ALA:HB1	1:B:430:PRO:CD	2.23	0.68
1:A:549:TRP:HZ3	1:A:556:LYS:O	1.76	0.68
1:B:417:LYS:O	1:B:497:LYS:HA	1.93	0.68
1:A:400:GLU:O	1:A:404:ILE:HG13	1.92	0.68
1:A:563:SER:O	1:A:567:VAL:HG23	1.94	0.68
1:A:459:LEU:HA	1:A:462:MET:HE3	1.74	0.68
1:A:413:LEU:HD13	1:A:473:LEU:CD2	2.23	0.68
1:B:398:MET:HE2	1:B:403:PHE:HB2	1.76	0.67
1:A:420:GLN:O	1:A:436:GLU:HG2	1.94	0.67
1:B:398:MET:SD	1:B:402:ASP:OD1	2.52	0.67
1:B:584:SER:H	1:B:587:VAL:HB	1.59	0.67
1:B:580:PRO:HG2	1:B:583:ALA:CB	2.10	0.67
1:A:422:TYR:CE1	1:A:436:GLU:HA	2.30	0.67
1:A:443:LEU:O	1:A:447:LEU:HG	1.93	0.67
1:B:529:VAL:HA	1:B:533:SER:HA	1.75	0.67
1:A:383:LEU:C	1:A:385:LYS:H	1.98	0.67
1:B:360:PRO:HA	1:B:427:GLU:HG3	1.76	0.66
1:B:398:MET:CE	1:B:403:PHE:HB2	2.26	0.66
1:A:360:PRO:HG2	1:A:362:GLU:CG	2.25	0.66
1:B:494:GLN:HE21	1:B:494:GLN:HA	1.60	0.66
1:A:480:HIS:CD2	1:A:501:PHE:HB3	2.31	0.66
1:B:485:ALA:N	1:B:547:LEU:HG	2.10	0.65
1:B:393:ILE:O	1:B:394:ARG:HG2	1.95	0.65
1:B:590:ILE:HD11	1:B:615:ILE:HD12	1.78	0.65
1:A:421:LEU:HD13	1:A:435:PHE:CE2	2.30	0.65
1:A:392:THR:HG22	1:A:432:CYS:HB3	1.77	0.65
1:A:493:ASN:O	1:A:495:VAL:N	2.29	0.65
1:B:419:VAL:CG2	1:B:499:SER:HB3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:THR:C	1:B:451:ARG:H	1.98	0.65
1:A:467:CYS:O	1:A:468:GLU:C	2.34	0.64
1:B:584:SER:HB2	1:B:587:VAL:HG23	1.80	0.64
1:B:546:VAL:O	1:B:549:TRP:HB3	1.97	0.64
1:B:382:TRP:C	1:B:384:ASN:H	2.01	0.64
1:B:538:LYS:HA	1:B:541:VAL:CG2	2.28	0.64
1:A:493:ASN:C	1:A:495:VAL:H	2.01	0.64
1:A:493:ASN:O	1:A:493:ASN:CG	2.36	0.63
1:A:586:HIS:HA	1:A:589:GLN:HG3	1.79	0.63
1:B:442:CYS:O	1:B:444:SER:N	2.31	0.63
1:A:486:ARG:NH2	1:A:524:TRP:CZ3	2.66	0.63
1:B:540:ASP:O	1:B:541:VAL:C	2.34	0.63
1:A:458:THR:HG22	1:A:462:MET:CE	2.28	0.63
1:B:401:GLU:HG3	1:B:402:ASP:N	2.13	0.63
1:A:540:ASP:O	1:A:543:SER:N	2.32	0.63
1:B:549:TRP:CE3	1:B:558:PRO:HB3	2.34	0.63
1:B:527:PRO:HA	1:B:530:PHE:CD1	2.33	0.63
1:A:429:ALA:CB	1:A:430:PRO:HD2	2.28	0.63
1:B:549:TRP:HZ3	1:B:556:LYS:O	1.82	0.62
1:B:460:LEU:HD11	1:B:612:LEU:HD22	1.81	0.62
1:A:590:ILE:O	1:A:593:HIS:N	2.32	0.62
1:B:443:LEU:HD11	1:B:447:LEU:HD21	1.81	0.62
1:B:428:GLN:HA	1:B:428:GLN:HE21	1.64	0.62
1:B:442:CYS:HA	1:B:489:LEU:HD23	1.82	0.62
1:B:540:ASP:O	1:B:542:TRP:N	2.32	0.62
1:B:540:ASP:O	1:B:544:PHE:N	2.33	0.62
1:B:501:PHE:N	1:B:501:PHE:CD2	2.61	0.62
1:A:550:GLU:O	1:A:551:VAL:C	2.38	0.62
1:A:549:TRP:CD2	1:A:577:LEU:HD13	2.34	0.62
1:B:415:HIS:ND1	1:B:416:PRO:HD2	2.15	0.62
1:A:449:THR:OG1	1:A:450:GLN:N	2.31	0.62
1:A:393:ILE:O	1:A:394:ARG:HG2	1.98	0.62
1:B:462:MET:O	1:B:465:ASP:HB2	2.00	0.61
1:A:450:GLN:O	1:A:453:LEU:CG	2.47	0.61
1:A:540:ASP:O	1:A:542:TRP:N	2.33	0.61
1:A:415:HIS:C	1:A:417:LYS:H	2.02	0.61
1:B:413:LEU:HB3	1:B:472:TYR:HE2	1.65	0.61
1:B:599:PRO:O	1:B:601:ASP:N	2.33	0.61
1:B:468:GLU:HG2	1:B:609:LEU:HD21	1.82	0.61
1:A:581:ARG:HG3	1:A:582:LEU:H	1.64	0.61
1:A:449:THR:C	1:A:451:ARG:H	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:THR:CG2	1:A:432:CYS:HB3	2.30	0.61
1:B:586:HIS:HA	1:B:589:GLN:CD	2.21	0.61
1:A:387:LYS:HE2	1:A:437:PHE:CD2	2.35	0.61
1:B:463:CYS:O	1:B:467:CYS:HB2	2.01	0.61
1:B:559:TYR:CE2	1:B:571:ILE:HD11	2.36	0.61
1:B:576:ARG:HE	1:B:595:TRP:HB3	1.66	0.61
1:B:399:SER:HB2	1:B:402:ASP:CB	2.30	0.61
1:A:470:MET:HE3	1:A:498:VAL:HG11	1.82	0.61
1:A:368:GLU:HG3	1:A:378:HIS:CE1	2.36	0.61
1:A:453:LEU:HD23	1:A:453:LEU:H	1.66	0.60
1:B:584:SER:HB2	1:B:587:VAL:CG2	2.31	0.60
1:A:574:GLY:HA2	1:A:576:ARG:NH1	2.16	0.60
1:B:458:THR:O	1:B:462:MET:HG3	2.01	0.60
1:B:426:LEU:C	1:B:428:GLN:H	2.04	0.60
1:A:417:LYS:C	1:A:497:LYS:HG2	2.22	0.60
1:A:357:VAL:O	1:A:357:VAL:HG13	2.01	0.60
1:A:546:VAL:O	1:A:549:TRP:HB3	2.01	0.59
1:A:563:SER:O	1:A:566:GLU:HB3	2.02	0.59
1:B:357:VAL:HG13	1:B:357:VAL:O	2.02	0.59
1:B:481:ARG:O	1:B:482:ASP:HB2	2.01	0.59
1:A:392:THR:HA	1:A:432:CYS:CB	2.30	0.59
1:A:580:PRO:O	1:A:583:ALA:N	2.34	0.59
1:A:460:LEU:HD23	1:A:616:ALA:HA	1.83	0.59
1:A:413:LEU:HD13	1:A:473:LEU:HD22	1.82	0.59
1:A:368:GLU:HG3	1:A:378:HIS:NE2	2.17	0.59
1:B:443:LEU:O	1:B:447:LEU:HG	2.02	0.59
1:B:549:TRP:CZ3	1:B:558:PRO:HB3	2.37	0.59
1:A:481:ARG:O	1:A:482:ASP:HB2	2.02	0.59
1:B:459:LEU:HD23	1:B:462:MET:CE	2.33	0.59
1:B:360:PRO:HD2	1:B:362:GLU:OE1	2.03	0.58
1:B:459:LEU:HD22	1:B:551:VAL:CG1	2.33	0.58
1:B:401:GLU:HG3	1:B:402:ASP:H	1.69	0.58
1:B:553:SER:O	1:B:555:GLY:N	2.36	0.58
1:B:415:HIS:CE1	1:B:416:PRO:HD2	2.38	0.58
1:B:428:GLN:O	1:B:429:ALA:CB	2.50	0.58
1:A:429:ALA:CB	1:A:430:PRO:CD	2.81	0.58
1:A:433:LEU:HD23	1:A:435:PHE:HZ	1.67	0.58
1:A:464:LEU:CD2	1:A:612:LEU:HB2	2.29	0.58
1:B:442:CYS:HA	1:B:489:LEU:HA	1.86	0.58
1:A:611:GLN:O	1:A:614:GLU:HB2	2.05	0.57
1:B:471:ALA:O	1:B:474:GLU:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:MET:O	1:A:595:TRP:CD2	2.57	0.57
1:B:452:GLY:C	1:B:454:PHE:H	2.08	0.57
1:A:452:GLY:C	1:A:454:PHE:H	2.05	0.57
1:A:552:PHE:CD2	1:A:583:ALA:HA	2.40	0.57
1:A:413:LEU:HB3	1:A:472:TYR:HE2	1.69	0.57
1:B:541:VAL:HG22	1:B:605:PHE:CE1	2.39	0.57
1:A:363:LEU:N	1:A:363:LEU:HD23	2.19	0.57
1:B:493:ASN:C	1:B:495:VAL:H	2.07	0.57
1:A:366:VAL:HG23	1:A:380:GLY:HA2	1.86	0.57
1:B:538:LYS:HA	1:B:541:VAL:HG23	1.87	0.56
1:B:542:TRP:C	1:B:544:PHE:H	2.07	0.56
1:B:523:LYS:HD3	1:B:558:PRO:O	2.04	0.56
1:A:368:GLU:OE2	1:A:376:LEU:HD13	2.05	0.56
1:B:444:SER:HB2	1:B:486:ARG:HA	1.87	0.56
1:B:486:ARG:NH2	1:B:524:TRP:CZ3	2.73	0.56
1:B:563:SER:O	1:B:566:GLU:HB3	2.05	0.56
1:B:429:ALA:CB	1:B:430:PRO:HD2	2.28	0.56
1:B:450:GLN:O	1:B:454:PHE:CE1	2.58	0.56
1:A:562:ARG:NH1	1:A:575:PHE:CE2	2.73	0.56
1:A:382:TRP:C	1:A:384:ASN:H	2.08	0.56
1:B:425:CYS:C	1:B:427:GLU:H	2.08	0.56
1:A:542:TRP:O	1:A:545:GLY:N	2.37	0.56
1:A:562:ARG:NH1	1:A:575:PHE:HE2	2.03	0.56
1:A:389:ALA:HB2	1:A:437:PHE:HD1	1.71	0.56
1:B:382:TRP:C	1:B:384:ASN:N	2.59	0.56
1:B:464:LEU:O	1:B:468:GLU:HG3	2.05	0.56
1:B:440:HIS:CD2	1:B:491:GLY:O	2.58	0.56
1:A:606:SER:O	1:A:610:ARG:HD2	2.06	0.56
1:B:464:LEU:CD2	1:B:609:LEU:HD12	2.35	0.56
1:A:424:VAL:HG13	1:A:433:LEU:CD1	2.35	0.56
1:A:475:GLU:C	1:A:477:CYS:N	2.51	0.56
1:A:472:TYR:O	1:A:476:ALA:N	2.39	0.56
1:A:428:GLN:NE2	1:A:428:GLN:HA	2.21	0.56
1:A:421:LEU:HD12	1:A:434:VAL:O	2.05	0.56
1:B:542:TRP:C	1:B:544:PHE:N	2.59	0.56
1:B:544:PHE:O	1:B:548:MET:HB2	2.06	0.56
1:B:492:GLU:O	1:B:493:ASN:OD1	2.24	0.56
1:B:426:LEU:HA	1:B:431:ILE:HG23	1.88	0.55
1:B:537:SER:O	1:B:541:VAL:HG23	2.07	0.55
1:A:398:MET:HG3	1:A:402:ASP:HB3	1.88	0.55
1:B:459:LEU:HD22	1:B:551:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:THR:HA	1:B:432:CYS:CB	2.19	0.55
1:B:449:THR:O	1:B:451:ARG:N	2.39	0.55
1:B:493:ASN:CG	1:B:493:ASN:O	2.45	0.55
1:B:546:VAL:O	1:B:547:LEU:C	2.42	0.55
1:B:605:PHE:HA	1:B:608:LEU:HD12	1.88	0.55
1:B:617:GLU:O	1:B:618:SER:CB	2.54	0.55
1:A:450:GLN:HG3	1:A:453:LEU:HD11	1.88	0.55
1:A:417:LYS:CA	1:A:497:LYS:HG2	2.36	0.55
1:B:527:PRO:HA	1:B:530:PHE:CE1	2.41	0.55
1:A:547:LEU:O	1:A:550:GLU:N	2.39	0.55
1:A:551:VAL:HG12	1:A:552:PHE:N	2.20	0.55
1:B:482:ASP:CG	1:B:482:ASP:O	2.45	0.55
1:A:586:HIS:ND1	1:A:589:GLN:OE1	2.40	0.55
1:B:468:GLU:CG	1:B:609:LEU:HD11	2.36	0.54
1:B:449:THR:C	1:B:451:ARG:N	2.61	0.54
1:A:417:LYS:HA	1:A:497:LYS:HG2	1.90	0.54
1:B:440:HIS:HD2	1:B:491:GLY:O	1.89	0.54
1:B:492:GLU:O	1:B:493:ASN:HB3	2.08	0.54
1:A:528:GLU:OE2	1:A:602:ARG:NH2	2.36	0.54
1:B:440:HIS:HB2	1:B:490:VAL:HB	1.88	0.54
1:B:451:ARG:HG2	1:B:452:GLY:N	2.21	0.54
1:A:581:ARG:HG3	1:A:582:LEU:N	2.22	0.54
1:A:560:GLU:O	1:A:562:ARG:N	2.35	0.54
1:A:382:TRP:C	1:A:384:ASN:N	2.60	0.54
1:A:536:SER:C	1:A:538:LYS:H	2.11	0.54
1:B:404:ILE:HG22	1:B:408:GLU:OE1	2.07	0.54
1:B:459:LEU:HD23	1:B:462:MET:HE3	1.89	0.54
1:B:460:LEU:HD23	1:B:616:ALA:HA	1.90	0.54
1:A:501:PHE:CD2	1:A:501:PHE:N	2.66	0.54
1:B:383:LEU:O	1:B:384:ASN:CB	2.56	0.54
1:B:492:GLU:H	1:B:492:GLU:CD	2.11	0.54
1:A:479:ILE:CD1	1:A:537:SER:HB2	2.38	0.54
1:B:567:VAL:HG12	1:B:571:ILE:HD12	1.90	0.54
1:A:548:MET:O	1:A:549:TRP:C	2.45	0.54
1:A:420:GLN:HB2	1:A:436:GLU:OE2	2.08	0.54
1:B:590:ILE:HD11	1:B:615:ILE:CD1	2.37	0.54
1:B:574:GLY:HA2	1:B:576:ARG:HH12	1.73	0.54
1:B:492:GLU:O	1:B:493:ASN:CB	2.56	0.54
1:B:558:PRO:HB2	1:B:559:TYR:CE1	2.43	0.53
1:B:449:THR:OG1	1:B:450:GLN:N	2.40	0.53
1:A:568:VAL:O	1:A:572:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLU:O	1:A:493:ASN:OD1	2.27	0.53
1:B:540:ASP:C	1:B:542:TRP:N	2.61	0.53
1:A:569:GLU:O	1:A:572:SER:N	2.42	0.53
1:B:598:ARG:O	1:B:602:ARG:HG3	2.08	0.53
1:B:416:PRO:O	1:B:417:LYS:HE3	2.09	0.53
1:A:523:LYS:HD3	1:A:558:PRO:O	2.07	0.53
1:B:498:VAL:HG12	1:B:499:SER:N	2.23	0.53
1:A:428:GLN:HA	1:A:428:GLN:HE21	1.71	0.53
1:A:470:MET:SD	1:A:483:LEU:HD22	2.48	0.53
1:A:459:LEU:CA	1:A:462:MET:HE3	2.38	0.53
1:B:580:PRO:O	1:B:583:ALA:HB3	2.08	0.53
1:A:590:ILE:HD11	1:A:615:ILE:HD12	1.91	0.53
1:B:479:ILE:O	1:B:481:ARG:HG3	2.09	0.53
1:A:479:ILE:HD12	1:A:537:SER:N	2.24	0.53
1:A:401:GLU:CG	1:A:402:ASP:H	2.15	0.52
1:B:481:ARG:O	1:B:482:ASP:CB	2.56	0.52
1:B:401:GLU:CG	1:B:402:ASP:H	2.22	0.52
1:B:547:LEU:O	1:B:550:GLU:N	2.42	0.52
1:B:552:PHE:C	1:B:554:GLU:N	2.59	0.52
1:A:425:CYS:O	1:A:431:ILE:HA	2.08	0.52
1:A:617:GLU:O	1:A:618:SER:CB	2.53	0.52
1:B:606:SER:O	1:B:610:ARG:HD2	2.09	0.52
1:A:586:HIS:HA	1:A:589:GLN:CG	2.39	0.52
1:A:379:LEU:HD12	1:A:380:GLY:N	2.23	0.52
1:A:464:LEU:HD23	1:A:612:LEU:HD12	1.91	0.52
1:A:546:VAL:CG1	1:A:558:PRO:HG3	2.40	0.52
1:B:438:MET:HE1	1:B:491:GLY:HA3	1.90	0.52
1:A:536:SER:O	1:A:537:SER:HB3	2.08	0.52
1:A:462:MET:O	1:A:465:ASP:HB2	2.10	0.52
1:A:532:PHE:CE2	1:A:534:ARG:NH2	2.77	0.52
1:A:562:ARG:CZ	1:A:575:PHE:CE2	2.93	0.52
1:A:438:MET:CE	1:A:491:GLY:HA3	2.39	0.52
1:A:392:THR:CA	1:A:432:CYS:HB3	2.35	0.52
1:B:452:GLY:O	1:B:454:PHE:N	2.43	0.51
1:B:425:CYS:C	1:B:427:GLU:N	2.62	0.51
1:B:421:LEU:HD11	1:B:433:LEU:HG	1.91	0.51
1:A:419:VAL:HG21	1:A:489:LEU:HD12	1.92	0.51
1:A:382:TRP:CD2	1:A:383:LEU:HG	2.45	0.51
1:B:459:LEU:HB3	1:B:551:VAL:CG1	2.40	0.51
1:B:558:PRO:C	1:B:559:TYR:CD1	2.84	0.51
1:B:401:GLU:CG	1:B:402:ASP:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:C	1:B:437:PHE:HB2	2.31	0.51
1:A:522:VAL:HG13	1:A:530:PHE:CD2	2.45	0.51
1:B:579:LYS:HA	1:B:588:TYR:CE1	2.45	0.51
1:B:454:PHE:N	1:B:454:PHE:CD1	2.78	0.51
1:A:428:GLN:O	1:A:429:ALA:HB3	2.11	0.51
1:A:398:MET:SD	1:A:402:ASP:OD1	2.69	0.51
1:B:363:LEU:HD13	1:B:390:ILE:HD13	1.91	0.51
1:A:523:LYS:NZ	1:A:557:ILE:CG2	2.74	0.51
1:A:549:TRP:CE3	1:A:558:PRO:HB3	2.46	0.51
1:B:413:LEU:HB3	1:B:472:TYR:CE2	2.45	0.51
1:B:473:LEU:O	1:B:478:VAL:N	2.43	0.51
1:A:375:GLY:CA	1:A:392:THR:O	2.57	0.50
1:A:549:TRP:CZ3	1:A:556:LYS:O	2.62	0.50
1:B:421:LEU:HD12	1:B:434:VAL:C	2.31	0.50
1:B:442:CYS:O	1:B:443:LEU:C	2.49	0.50
1:A:449:THR:C	1:A:451:ARG:N	2.65	0.50
1:B:600:GLU:HG2	1:B:601:ASP:N	2.27	0.50
1:A:570:ASP:O	1:A:575:PHE:HB3	2.11	0.50
1:A:363:LEU:HA	1:A:381:TYR:O	2.11	0.50
1:B:558:PRO:HB2	1:B:559:TYR:CD1	2.46	0.50
1:B:385:LYS:HE2	1:B:385:LYS:HA	1.94	0.50
1:A:459:LEU:HA	1:A:462:MET:CE	2.40	0.50
1:A:586:HIS:HA	1:A:589:GLN:CD	2.32	0.50
1:B:536:SER:H	1:B:539:SER:CB	2.24	0.50
1:B:547:LEU:C	1:B:547:LEU:HD23	2.31	0.50
1:B:470:MET:O	1:B:471:ALA:C	2.50	0.50
1:A:536:SER:O	1:A:538:LYS:N	2.42	0.50
1:A:417:LYS:O	1:A:497:LYS:CA	2.58	0.50
1:A:385:LYS:HA	1:A:385:LYS:HE2	1.94	0.50
1:B:475:GLU:O	1:B:477:CYS:N	2.44	0.49
1:B:426:LEU:O	1:B:428:GLN:N	2.38	0.49
1:A:607:ARG:HB2	1:A:607:ARG:NH1	2.09	0.49
1:B:460:LEU:C	1:B:462:MET:H	2.15	0.49
1:B:462:MET:O	1:B:465:ASP:N	2.44	0.49
1:A:421:LEU:HA	1:A:435:PHE:HA	1.95	0.49
1:B:438:MET:CE	1:B:491:GLY:HA3	2.42	0.49
1:A:525:ALA:HB3	1:A:530:PHE:HE2	1.77	0.49
1:A:413:LEU:HB3	1:A:472:TYR:CE2	2.47	0.49
1:B:592:ASN:HA	1:B:595:TRP:HB2	1.95	0.49
1:A:421:LEU:HD11	1:A:433:LEU:HG	1.95	0.49
1:B:420:GLN:O	1:B:436:GLU:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:TRP:CG	1:A:577:LEU:HD13	2.48	0.49
1:A:576:ARG:N	1:A:576:ARG:HD2	2.27	0.49
1:A:584:SER:O	1:A:587:VAL:HB	2.13	0.49
1:B:443:LEU:O	1:B:443:LEU:HD12	2.13	0.49
1:A:421:LEU:HD13	1:A:435:PHE:CG	2.48	0.49
1:B:421:LEU:HD12	1:B:435:PHE:HA	1.93	0.49
1:A:540:ASP:C	1:A:542:TRP:N	2.66	0.49
1:B:388:VAL:CA	1:B:437:PHE:HB2	2.43	0.49
1:A:387:LYS:HE2	1:A:437:PHE:CE2	2.48	0.49
1:A:467:CYS:O	1:A:470:MET:N	2.45	0.49
1:A:474:GLU:OE1	1:A:605:PHE:N	2.44	0.49
1:A:562:ARG:NH2	1:A:575:PHE:CZ	2.80	0.48
1:A:422:TYR:HE1	1:A:436:GLU:CA	2.24	0.48
1:B:442:CYS:CA	1:B:489:LEU:HD23	2.42	0.48
1:B:442:CYS:SG	1:B:444:SER:HB3	2.54	0.48
1:B:536:SER:O	1:B:537:SER:HB3	2.14	0.48
1:B:586:HIS:HA	1:B:589:GLN:CG	2.44	0.48
1:B:421:LEU:HD12	1:B:435:PHE:N	2.28	0.48
1:A:562:ARG:HA	1:A:566:GLU:OE1	2.14	0.48
1:A:383:LEU:C	1:A:385:LYS:N	2.65	0.48
1:B:401:GLU:O	1:B:404:ILE:HB	2.13	0.48
1:B:454:PHE:N	1:B:454:PHE:HD1	2.11	0.48
1:A:452:GLY:C	1:A:454:PHE:N	2.66	0.48
1:A:426:LEU:C	1:A:428:GLN:H	2.17	0.48
1:A:574:GLY:HA2	1:A:576:ARG:HH12	1.77	0.48
1:B:569:GLU:O	1:B:570:ASP:C	2.52	0.48
1:A:368:GLU:HG3	1:A:378:HIS:CD2	2.49	0.48
1:A:391:LYS:O	1:A:433:LEU:N	2.36	0.48
1:A:402:ASP:O	1:A:405:GLU:HB3	2.13	0.48
1:A:474:GLU:CD	1:A:605:PHE:HB2	2.34	0.48
1:B:398:MET:HG2	1:B:403:PHE:CB	2.44	0.48
1:A:552:PHE:C	1:A:554:GLU:H	2.15	0.48
1:B:586:HIS:O	1:B:589:GLN:HB2	2.14	0.48
1:A:464:LEU:CD2	1:A:609:LEU:HD12	2.39	0.48
1:B:580:PRO:O	1:B:583:ALA:N	2.46	0.47
1:A:464:LEU:O	1:A:468:GLU:N	2.38	0.47
1:A:580:PRO:O	1:A:583:ALA:HB3	2.14	0.47
1:A:367:GLN:NE2	1:A:367:GLN:HA	2.28	0.47
1:B:541:VAL:O	1:B:544:PHE:HB3	2.14	0.47
1:B:421:LEU:HD12	1:B:435:PHE:CA	2.45	0.47
1:A:540:ASP:O	1:A:541:VAL:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:O	1:A:462:MET:HE3	2.14	0.47
1:B:451:ARG:O	1:B:453:LEU:HD23	2.14	0.47
1:A:584:SER:HB2	1:A:587:VAL:HG23	1.96	0.47
1:B:450:GLN:O	1:B:453:LEU:CG	2.49	0.47
1:B:419:VAL:HG23	1:B:498:VAL:O	2.14	0.47
1:B:428:GLN:HA	1:B:428:GLN:NE2	2.28	0.47
1:A:450:GLN:HB3	1:A:454:PHE:CZ	2.50	0.47
1:B:586:HIS:HA	1:B:589:GLN:HG3	1.96	0.47
1:B:417:LYS:O	1:B:497:LYS:CA	2.63	0.47
1:B:522:VAL:O	1:B:523:LYS:C	2.53	0.47
1:B:429:ALA:CB	1:B:430:PRO:CD	2.90	0.47
1:A:401:GLU:O	1:A:404:ILE:HB	2.14	0.46
1:A:558:PRO:HB2	1:A:559:TYR:CE1	2.51	0.46
1:A:471:ALA:O	1:A:474:GLU:HB3	2.15	0.46
1:A:591:MET:HB3	1:A:595:TRP:CZ3	2.51	0.46
1:B:493:ASN:O	1:B:495:VAL:N	2.47	0.46
1:B:443:LEU:HD11	1:B:447:LEU:CD2	2.45	0.46
1:A:563:SER:C	1:A:567:VAL:HG23	2.35	0.46
1:B:536:SER:O	1:B:538:LYS:N	2.43	0.46
1:A:553:SER:O	1:A:555:GLY:N	2.49	0.46
1:A:580:PRO:HG2	1:A:583:ALA:CB	2.36	0.46
1:A:415:HIS:C	1:A:417:LYS:N	2.68	0.46
1:B:417:LYS:O	1:B:498:VAL:N	2.45	0.46
1:B:468:GLU:O	1:B:469:GLY:C	2.53	0.46
1:A:473:LEU:HA	1:A:476:ALA:CB	2.42	0.46
1:B:452:GLY:C	1:B:454:PHE:N	2.67	0.46
1:A:360:PRO:HG2	1:A:362:GLU:CD	2.36	0.46
1:B:613:ALA:O	1:B:617:GLU:HG3	2.16	0.46
1:B:392:THR:HG22	1:B:432:CYS:SG	2.55	0.46
1:B:599:PRO:O	1:B:600:GLU:C	2.54	0.46
1:A:547:LEU:O	1:A:548:MET:C	2.53	0.46
1:B:403:PHE:HE2	1:B:426:LEU:HD22	1.81	0.46
1:A:598:ARG:HD3	1:A:600:GLU:OE2	2.16	0.46
1:A:558:PRO:HB2	1:A:559:TYR:CD1	2.51	0.46
1:A:419:VAL:HG12	1:A:419:VAL:O	2.14	0.46
1:A:442:CYS:CA	1:A:489:LEU:HD23	2.41	0.45
1:A:486:ARG:HG2	1:A:486:ARG:NH1	2.31	0.45
1:A:368:GLU:HG2	1:A:377:VAL:O	2.16	0.45
1:A:588:TYR:O	1:A:592:ASN:ND2	2.49	0.45
1:A:577:LEU:O	1:A:578:TYR:O	2.33	0.45
1:B:363:LEU:CD1	1:B:390:ILE:HD13	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD13	1:B:435:PHE:CD2	2.51	0.45
1:A:420:GLN:N	1:A:436:GLU:OE2	2.43	0.45
1:A:382:TRP:CG	1:A:383:LEU:HG	2.50	0.45
1:A:493:ASN:C	1:A:495:VAL:N	2.67	0.45
1:B:524:TRP:NE1	1:B:550:GLU:OE2	2.49	0.45
1:B:480:HIS:CG	1:B:501:PHE:HB3	2.50	0.45
1:A:479:ILE:HD12	1:A:537:SER:CA	2.47	0.45
1:A:438:MET:HE3	1:A:491:GLY:HA3	1.99	0.45
1:B:549:TRP:CD2	1:B:577:LEU:HD13	2.51	0.45
1:B:470:MET:HB2	1:B:605:PHE:CD2	2.52	0.45
1:B:383:LEU:C	1:B:385:LYS:H	2.20	0.45
1:B:450:GLN:C	1:B:454:PHE:HE1	2.20	0.45
1:A:393:ILE:HG22	1:A:394:ARG:N	2.32	0.45
1:A:459:LEU:HD11	1:A:582:LEU:HD13	1.98	0.45
1:B:562:ARG:NH2	1:B:575:PHE:CZ	2.84	0.45
1:B:569:GLU:O	1:B:572:SER:N	2.50	0.45
1:A:385:LYS:HD3	1:A:385:LYS:O	2.17	0.45
1:A:486:ARG:NH2	1:A:524:TRP:CH2	2.85	0.45
1:B:443:LEU:CD1	1:B:447:LEU:HG	2.47	0.45
1:B:601:ASP:N	1:B:601:ASP:OD1	2.49	0.45
1:A:561:ASN:C	1:A:562:ARG:HG3	2.36	0.44
1:B:529:VAL:HA	1:B:533:SER:CA	2.43	0.44
1:B:491:GLY:C	1:B:493:ASN:H	2.20	0.44
1:B:600:GLU:CG	1:B:601:ASP:OD1	2.54	0.44
1:B:405:GLU:O	1:B:408:GLU:HB2	2.18	0.44
1:B:428:GLN:NE2	1:B:428:GLN:CA	2.80	0.44
1:A:442:CYS:O	1:A:443:LEU:C	2.55	0.44
1:A:523:LYS:HZ2	1:A:557:ILE:CG2	2.30	0.44
1:A:443:LEU:HG	1:A:447:LEU:HD11	1.97	0.44
1:A:459:LEU:CD1	1:A:582:LEU:HD13	2.48	0.44
1:A:560:GLU:C	1:A:562:ARG:H	2.16	0.44
1:B:398:MET:HE3	1:B:403:PHE:HA	2.00	0.44
1:A:551:VAL:HG12	1:A:552:PHE:CD1	2.53	0.44
1:A:443:LEU:HG	1:A:447:LEU:CD1	2.48	0.44
1:B:547:LEU:O	1:B:548:MET:C	2.56	0.44
1:A:449:THR:O	1:A:451:ARG:N	2.50	0.44
1:A:568:VAL:O	1:A:569:GLU:C	2.56	0.44
1:B:529:VAL:O	1:B:529:VAL:HG12	2.17	0.44
1:B:590:ILE:O	1:B:593:HIS:HB2	2.18	0.44
1:B:610:ARG:O	1:B:613:ALA:CB	2.57	0.43
1:A:417:LYS:HA	1:A:417:LYS:HD3	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:HD23	1:B:616:ALA:CA	2.48	0.43
1:B:476:ALA:O	1:B:477:CYS:C	2.57	0.43
1:B:394:ARG:O	1:B:395:GLU:HG3	2.19	0.43
1:B:402:ASP:O	1:B:405:GLU:HB3	2.18	0.43
1:A:552:PHE:HD2	1:A:583:ALA:HA	1.83	0.43
1:A:385:LYS:HD3	1:A:385:LYS:C	2.39	0.43
1:A:585:THR:O	1:A:589:GLN:HG3	2.18	0.43
1:A:398:MET:SD	1:A:403:PHE:HB2	2.58	0.43
1:B:474:GLU:CD	1:B:605:PHE:HB2	2.39	0.43
1:A:443:LEU:HD11	1:A:447:LEU:HD21	2.00	0.43
1:B:486:ARG:HH11	1:B:486:ARG:CG	2.31	0.43
1:B:484:ALA:HA	1:B:547:LEU:HB2	2.01	0.43
1:B:398:MET:HG2	1:B:403:PHE:HB3	1.99	0.43
1:A:607:ARG:CB	1:A:607:ARG:HH11	2.11	0.43
1:A:388:VAL:HG21	1:A:434:VAL:HG11	2.01	0.43
1:A:398:MET:SD	1:A:403:PHE:CA	3.06	0.43
1:B:560:GLU:C	1:B:562:ARG:H	2.22	0.43
1:B:483:LEU:HD21	1:B:544:PHE:HD1	1.82	0.43
1:A:468:GLU:O	1:A:469:GLY:C	2.57	0.43
1:A:599:PRO:O	1:A:601:ASP:N	2.52	0.43
1:A:560:GLU:C	1:A:562:ARG:N	2.72	0.43
1:B:476:ALA:O	1:B:477:CYS:O	2.37	0.43
1:B:484:ALA:C	1:B:547:LEU:HG	2.40	0.43
1:B:535:TYR:HA	1:B:539:SER:HB3	2.01	0.43
1:B:464:LEU:CD2	1:B:612:LEU:HB2	2.40	0.43
1:A:563:SER:O	1:A:564:ASN:C	2.56	0.42
1:A:569:GLU:O	1:A:570:ASP:C	2.57	0.42
1:A:380:GLY:O	1:A:381:TYR:CD1	2.72	0.42
1:B:406:GLU:HG2	1:B:410:MET:CE	2.49	0.42
1:B:523:LYS:HE2	1:B:559:TYR:O	2.19	0.42
1:B:401:GLU:CA	1:B:404:ILE:HD12	2.46	0.42
1:A:553:SER:O	1:A:554:GLU:C	2.57	0.42
1:B:474:GLU:OE1	1:B:605:PHE:HD1	2.02	0.42
1:B:427:GLU:O	1:B:428:GLN:O	2.36	0.42
1:B:382:TRP:O	1:B:384:ASN:N	2.52	0.42
1:A:598:ARG:HB2	1:A:601:ASP:OD2	2.19	0.42
1:A:492:GLU:O	1:A:493:ASN:CB	2.67	0.42
1:B:590:ILE:O	1:B:591:MET:C	2.57	0.42
1:A:382:TRP:O	1:A:384:ASN:N	2.53	0.42
1:A:522:VAL:HG13	1:A:530:PHE:CE2	2.54	0.42
1:A:552:PHE:C	1:A:554:GLU:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:VAL:HG12	1:B:499:SER:H	1.82	0.42
1:A:422:TYR:CE1	1:A:436:GLU:CA	3.01	0.42
1:B:579:LYS:HA	1:B:588:TYR:CD1	2.54	0.42
1:B:609:LEU:O	1:B:613:ALA:HB2	2.19	0.42
1:B:415:HIS:ND1	1:B:416:PRO:CD	2.81	0.42
1:A:493:ASN:ND2	1:A:493:ASN:O	2.51	0.42
1:A:367:GLN:HE21	1:A:367:GLN:HA	1.83	0.42
1:B:483:LEU:HD23	1:B:544:PHE:HA	2.00	0.42
1:B:567:VAL:O	1:B:568:VAL:C	2.58	0.42
1:B:360:PRO:CG	1:B:362:GLU:CD	2.88	0.42
1:B:426:LEU:C	1:B:428:GLN:N	2.71	0.42
1:A:483:LEU:HD21	1:A:544:PHE:CD1	2.55	0.42
1:A:428:GLN:NE2	1:A:428:GLN:CA	2.80	0.42
1:B:562:ARG:NH2	1:B:575:PHE:CE2	2.88	0.42
1:A:476:ALA:O	1:A:477:CYS:C	2.57	0.42
1:A:462:MET:HB3	1:A:496:ILE:HG13	2.01	0.42
1:B:494:GLN:NE2	1:B:494:GLN:HA	2.32	0.42
1:B:599:PRO:HA	1:B:602:ARG:NE	2.34	0.42
1:A:452:GLY:N	1:A:554:GLU:OE2	2.45	0.42
1:A:590:ILE:H	1:A:590:ILE:HG13	1.65	0.42
1:A:458:THR:C	1:A:462:MET:HE3	2.40	0.42
1:B:560:GLU:O	1:B:562:ARG:N	2.49	0.42
1:A:486:ARG:HG3	1:A:486:ARG:O	2.20	0.42
1:B:470:MET:HE2	1:B:473:LEU:HD12	2.02	0.42
1:A:590:ILE:O	1:A:591:MET:C	2.58	0.42
1:B:570:ASP:O	1:B:573:THR:OG1	2.37	0.42
1:A:367:GLN:HE21	1:A:367:GLN:CA	2.31	0.42
1:A:558:PRO:HB2	1:A:577:LEU:HD11	2.01	0.41
1:A:475:GLU:O	1:A:475:GLU:HG2	2.19	0.41
1:B:527:PRO:HD3	1:B:542:TRP:CZ3	2.56	0.41
1:B:403:PHE:CE2	1:B:426:LEU:HD22	2.54	0.41
1:A:600:GLU:HG2	1:A:601:ASP:N	2.36	0.41
1:B:549:TRP:O	1:B:550:GLU:C	2.59	0.41
1:B:611:GLN:O	1:B:614:GLU:N	2.53	0.41
1:A:388:VAL:HG21	1:A:434:VAL:CG1	2.50	0.41
1:A:462:MET:O	1:A:465:ASP:N	2.52	0.41
1:A:579:LYS:HE2	1:A:588:TYR:HB2	2.01	0.41
1:A:406:GLU:HG2	1:A:410:MET:CE	2.50	0.41
1:A:548:MET:O	1:A:551:VAL:HB	2.20	0.41
1:A:580:PRO:O	1:A:583:ALA:CB	2.68	0.41
1:B:587:VAL:C	1:B:589:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:PHE:CD2	1:A:534:ARG:NH2	2.88	0.41
1:A:382:TRP:NE1	1:A:383:LEU:HD21	2.36	0.41
1:B:548:MET:O	1:B:551:VAL:HB	2.20	0.41
1:A:401:GLU:O	1:A:402:ASP:C	2.59	0.41
1:A:450:GLN:O	1:A:451:ARG:C	2.58	0.41
1:A:577:LEU:C	1:A:578:TYR:O	2.58	0.41
1:A:484:ALA:O	1:A:485:ALA:C	2.56	0.41
1:B:563:SER:O	1:B:567:VAL:HG23	2.21	0.41
1:B:413:LEU:HD13	1:B:478:VAL:HG21	2.02	0.41
1:B:459:LEU:O	1:B:462:MET:HB2	2.21	0.41
1:A:401:GLU:HA	1:A:404:ILE:HD12	2.02	0.41
1:B:499:SER:O	1:B:500:ASP:HB2	2.21	0.41
1:A:444:SER:HB2	1:A:486:ARG:HA	2.03	0.41
1:A:535:TYR:HA	1:A:539:SER:CB	2.50	0.41
1:B:451:ARG:HG2	1:B:452:GLY:H	1.82	0.41
1:A:483:LEU:HD21	1:A:544:PHE:HD1	1.85	0.41
1:B:570:ASP:C	1:B:575:PHE:HB3	2.40	0.41
1:B:472:TYR:O	1:B:476:ALA:N	2.33	0.41
1:B:429:ALA:O	1:B:431:ILE:N	2.54	0.41
1:A:383:LEU:O	1:A:385:LYS:N	2.54	0.41
1:A:535:TYR:HA	1:A:539:SER:HB3	2.02	0.41
1:B:528:GLU:CD	1:B:528:GLU:H	2.23	0.41
1:B:547:LEU:C	1:B:547:LEU:CD2	2.88	0.41
1:B:401:GLU:O	1:B:402:ASP:C	2.60	0.41
1:A:458:THR:O	1:A:462:MET:HG3	2.21	0.41
1:A:568:VAL:O	1:A:572:SER:N	2.48	0.41
1:B:604:ALA:O	1:B:605:PHE:C	2.58	0.40
1:B:428:GLN:O	1:B:429:ALA:HB3	2.21	0.40
1:A:421:LEU:HD12	1:A:435:PHE:HA	2.04	0.40
1:A:379:LEU:HD12	1:A:380:GLY:H	1.85	0.40
1:B:413:LEU:HA	1:B:472:TYR:OH	2.21	0.40
1:B:415:HIS:C	1:B:417:LYS:H	2.23	0.40
1:A:602:ARG:O	1:A:603:PRO:O	2.38	0.40
1:B:493:ASN:C	1:B:495:VAL:N	2.74	0.40
1:A:536:SER:C	1:A:538:LYS:N	2.74	0.40
1:A:451:ARG:HG2	1:A:452:GLY:N	2.36	0.40
1:B:492:GLU:CD	1:B:492:GLU:N	2.73	0.40
1:B:580:PRO:O	1:B:583:ALA:CB	2.70	0.40
1:A:426:LEU:HA	1:A:431:ILE:HG23	2.02	0.40
1:A:486:ARG:HG2	1:A:486:ARG:HH11	1.86	0.40
1:B:479:ILE:HG22	1:B:481:ARG:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:GLU:OE2	1:B:581:ARG:N[1_544]	2.15	0.05

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	241/264 (91%)	157 (65%)	53 (22%)	31 (13%)	0 2
1	B	241/264 (91%)	146 (61%)	54 (22%)	41 (17%)	0 1
All	All	482/528 (91%)	303 (63%)	107 (22%)	72 (15%)	0 1

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PHE
1	A	429	ALA
1	A	444	SER
1	A	453	LEU
1	A	482	ASP
1	A	554	GLU
1	A	603	PRO
1	A	618	SER
1	B	369	ILE
1	B	374	PHE
1	B	395	GLU
1	B	428	GLN
1	B	429	ALA
1	B	443	LEU
1	B	448	ARG
1	B	482	ASP
1	B	493	ASN

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Mol	Chain	Res	Type
1	B	554	GLU
1	B	600	GLU
1	B	618	SER
1	A	394	ARG
1	A	416	PRO
1	A	441	GLY
1	A	494	GLN
1	A	536	SER
1	A	541	VAL
1	A	578	TYR
1	A	600	GLU
1	B	394	ARG
1	B	427	GLU
1	B	444	SER
1	B	449	THR
1	B	451	ARG
1	B	453	LEU
1	B	492	GLU
1	B	536	SER
1	B	541	VAL
1	A	405	GLU
1	A	451	ARG
1	A	566	GLU
1	B	441	GLY
1	B	578	TYR
1	B	599	PRO
1	B	614	GLU
1	A	428	GLN
1	A	493	ASN
1	A	533	SER
1	A	599	PRO
1	B	477	CYS
1	B	481	ARG
1	B	494	GLN
1	B	501	PHE
1	B	569	GLU
1	A	369	ILE
1	A	393	ILE
1	A	427	GLU
1	A	561	ASN
1	A	574	GLY
1	A	614	GLU

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Mol	Chain	Res	Type
1	B	393	ILE
1	B	561	ASN
1	B	566	GLU
1	A	551	VAL
1	B	360	PRO
1	B	402	ASP
1	B	416	PRO
1	B	450	GLN
1	B	603	PRO
1	A	419	VAL
1	B	388	VAL
1	B	568	VAL
1	B	469	GLY

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	214/232 (92%)	194 (91%)	20 (9%)	11 41
1	B	214/232 (92%)	192 (90%)	22 (10%)	9 36
All	All	428/464 (92%)	386 (90%)	42 (10%)	10 38

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	LEU
1	A	369	ILE
1	A	374	PHE
1	A	385	LYS
1	A	394	ARG
1	A	403	PHE
1	A	409	VAL
1	A	414	SER
1	A	425	CYS
1	A	449	THR

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Mol	Chain	Res	Type
1	A	453	LEU
1	A	486	ARG
1	A	493	ASN
1	A	495	VAL
1	A	501	PHE
1	A	528	GLU
1	A	531	SER
1	A	597	GLU
1	A	601	ASP
1	A	607	ARG
1	B	359	ASP
1	B	363	LEU
1	B	367	GLN
1	B	368	GLU
1	B	374	PHE
1	B	385	LYS
1	B	403	PHE
1	B	428	GLN
1	B	432	CYS
1	B	449	THR
1	B	450	GLN
1	B	453	LEU
1	B	454	PHE
1	B	475	GLU
1	B	486	ARG
1	B	494	GLN
1	B	501	PHE
1	B	528	GLU
1	B	597	GLU
1	B	601	ASP
1	B	607	ARG
1	B	610	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	A	428	GLN
1	A	440	HIS
1	A	487	ASN
1	A	493	ASN
1	A	494	GLN

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Mol	Chain	Res	Type
1	A	593	HIS
1	A	611	GLN
1	B	367	GLN
1	B	428	GLN
1	B	440	HIS
1	B	493	ASN
1	B	494	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.