Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:56 PM GMT

PDB ID	:	1D5F
Title	:	STRUCTURE OF AN E6AP-UBCH7 COMPLEX: INSIGHTS INTO THE UBIQUITINATION PATHWAY
Authors	:	Huang, L.; Kinnucan, E.; Wang, G.; Beaudenon, S.; Howley, P.M.; Huibregtse, J.M.; Pavletich, N.P.
Deposited on	:	1999-10-07
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
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 (1)) were used in the production of this report:

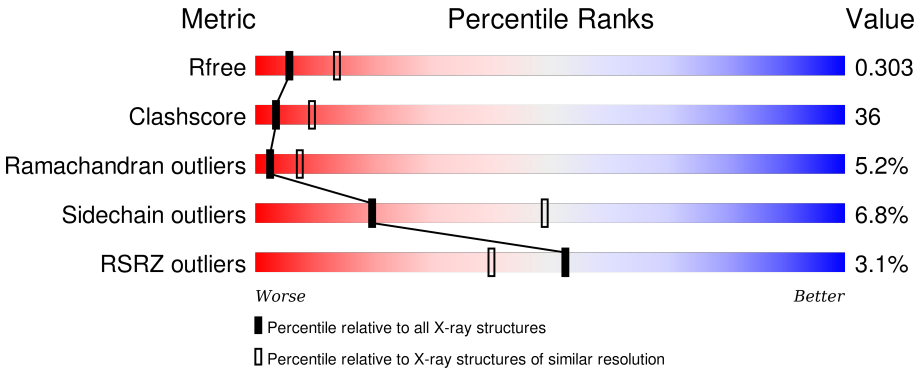
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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.

Mol	Chain	Length	Quality of chain
1	A	358	2% 44% 45% 9%
1	B	358	4% 44% 44% 9%
1	C	358	3% 45% 44% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8583 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 E6AP HECT CATALYTIC DOMAIN, E3 LIGASE.

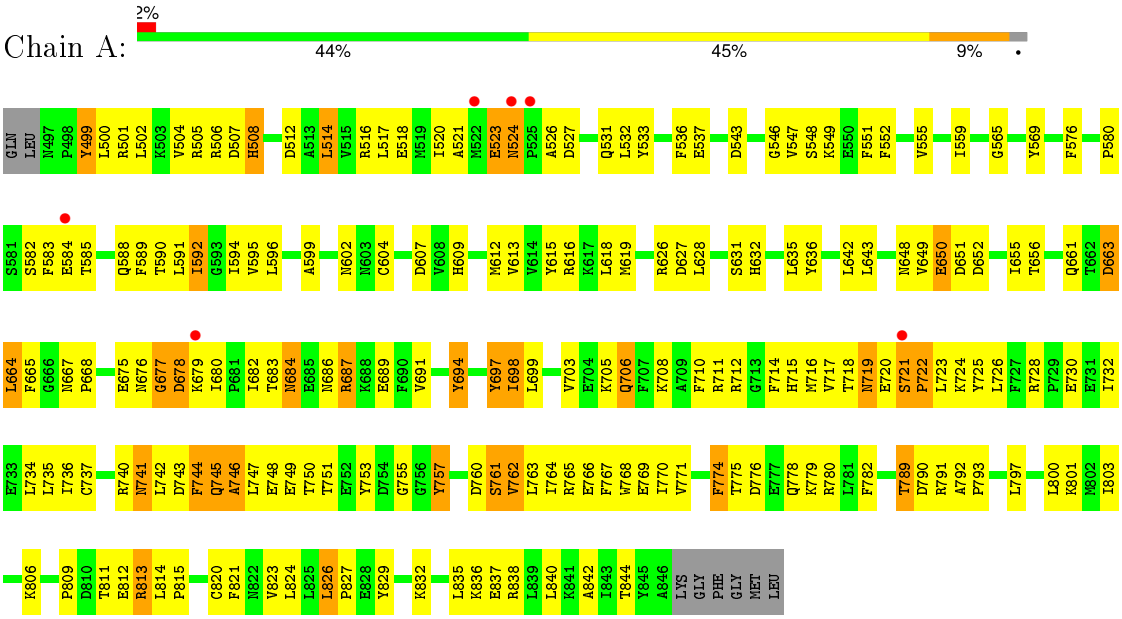
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2861	1839	467	541	14			
1	B	350	Total	C	N	O	S	0	0	0
			2861	1839	467	541	14			
1	C	350	Total	C	N	O	S	0	0	0
			2861	1839	467	541	14			

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.

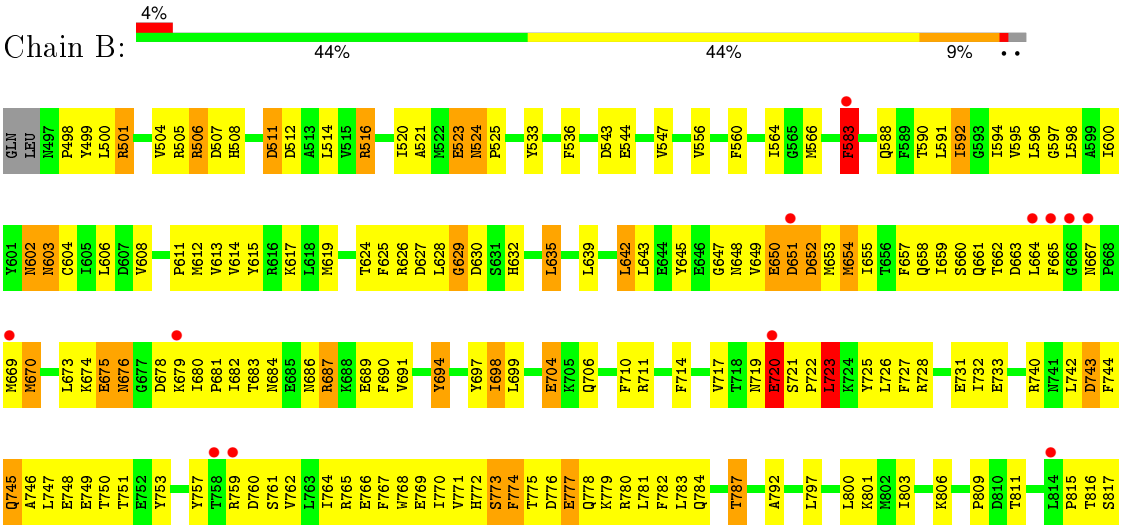
- Molecule 1: E6AP HECT CATALYTIC DOMAIN, E3 LIGASE

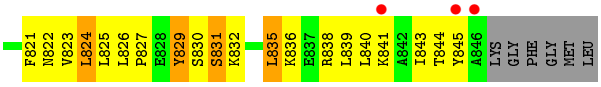
Chain A:



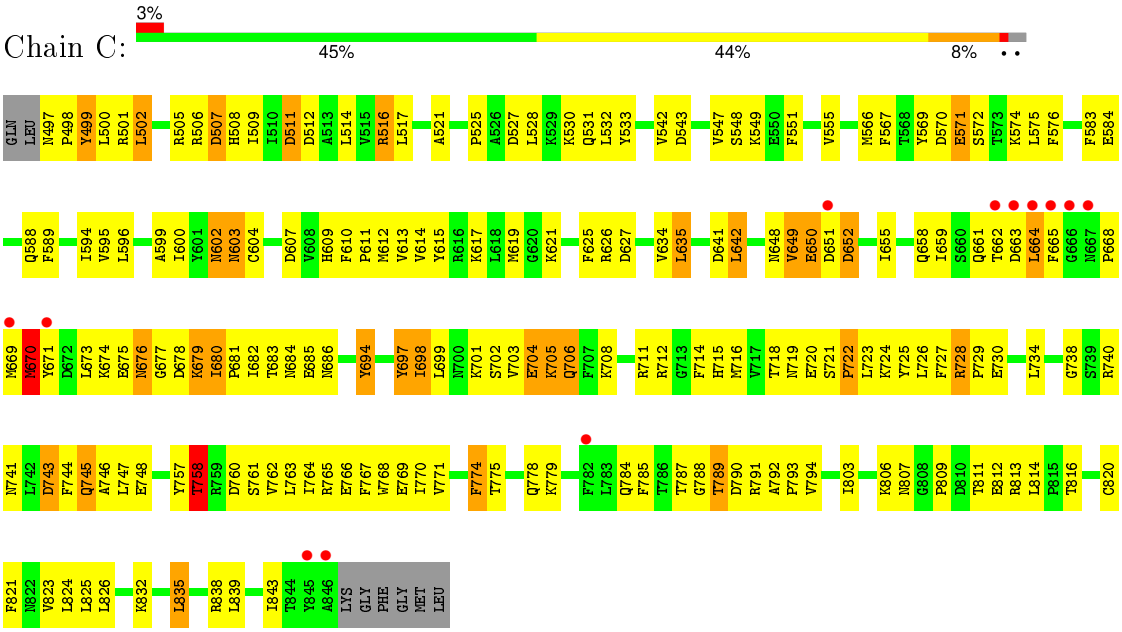
- Molecule 1: E6AP HECT CATALYTIC DOMAIN, E3 LIGASE

Chain B:





• Molecule 1: E6AP HECT CATALYTIC DOMAIN, E3 LIGASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.50Å 113.70Å 125.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	32190.0 (15.00-2.80) 97.7 (19.98-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.283 0.245 , 0.303	Depositor DCC
R_{free} test set	1789 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 35410 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8583	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/2923	0.76	2/3943 (0.1%)
1	B	0.43	0/2923	0.76	3/3943 (0.1%)
1	C	0.43	0/2923	0.76	4/3943 (0.1%)
All	All	0.43	0/8769	0.76	9/11829 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	745	GLN	N-CA-C	-9.32	85.82	111.00
1	C	745	GLN	N-CA-C	-9.22	86.09	111.00
1	A	745	GLN	N-CA-C	-7.69	90.23	111.00
1	B	723	LEU	N-CA-C	-7.36	91.13	111.00
1	A	697	TYR	N-CA-C	-5.97	94.87	111.00
1	C	602	ASN	N-CA-C	-5.61	95.85	111.00
1	C	697	TYR	N-CA-C	-5.50	96.14	111.00
1	B	583	PHE	N-CA-C	5.45	125.72	111.00
1	C	502	LEU	CA-CB-CG	5.38	127.68	115.30

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	2861	0	2827	208	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2861	0	2827	214	0
1	C	2861	0	2827	223	0
All	All	8583	0	8481	621	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 36.

All (621) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:ARG:HH11	1:C:728:ARG:HB3	1.06	1.12
1:C:516:ARG:HH11	1:C:516:ARG:HB2	1.28	0.98
1:C:517:LEU:HD13	1:C:594:ILE:HG21	1.49	0.94
1:C:814:LEU:HD23	1:C:838:ARG:HD3	1.50	0.94
1:C:649:VAL:H	1:C:684:ASN:HD21	1.03	0.93
1:B:625:PHE:HE2	1:C:542:VAL:HG11	1.34	0.93
1:C:728:ARG:NH1	1:C:728:ARG:HB3	1.83	0.91
1:B:583:PHE:HD2	1:B:583:PHE:N	1.69	0.91
1:C:728:ARG:HH11	1:C:728:ARG:CB	1.84	0.89
1:C:649:VAL:HG23	1:C:684:ASN:ND2	1.87	0.89
1:C:516:ARG:NH1	1:C:516:ARG:HB2	1.86	0.89
1:C:603:ASN:HD21	1:C:794:VAL:HB	1.36	0.88
1:A:683:THR:H	1:A:686:ASN:ND2	1.70	0.88
1:B:742:LEU:HD11	1:B:780:ARG:NH1	1.89	0.88
1:C:704:GLU:HG2	1:C:705:LYS:H	1.40	0.87
1:A:583:PHE:CD1	1:A:584:GLU:HG2	2.11	0.85
1:B:660:SER:HA	1:B:670:MET:HE2	1.59	0.85
1:B:683:THR:HG23	1:B:686:ASN:ND2	1.91	0.84
1:C:506:ARG:O	1:C:507:ASP:HB2	1.77	0.83
1:C:634:VAL:HG13	1:C:635:LEU:H	1.43	0.83
1:A:720:GLU:O	1:A:722:PRO:HD2	1.79	0.83
1:C:697:TYR:O	1:C:698:ILE:HB	1.80	0.82
1:A:649:VAL:H	1:A:684:ASN:HD21	1.28	0.81
1:B:592:ILE:HD13	1:B:592:ILE:O	1.81	0.81
1:C:649:VAL:H	1:C:684:ASN:ND2	1.79	0.81
1:B:816:THR:HG23	1:B:825:LEU:HD12	1.63	0.80
1:A:840:LEU:O	1:A:844:THR:HG22	1.81	0.80
1:C:728:ARG:NH1	1:C:729:PRO:HD2	1.96	0.80
1:B:775:THR:OG1	1:B:778:GLN:HG3	1.81	0.80
1:A:723:LEU:HG	1:A:732:ILE:HD11	1.63	0.80
1:A:728:ARG:HH21	1:B:603:ASN:HA	1.45	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:LEU:H	1:C:602:ASN:HD21	1.31	0.78
1:B:649:VAL:O	1:B:650:GLU:HB2	1.82	0.78
1:A:723:LEU:HG	1:A:732:ILE:CD1	2.13	0.78
1:B:613:VAL:HG22	1:B:627:ASP:HB3	1.66	0.78
1:C:745:GLN:O	1:C:746:ALA:HB3	1.83	0.78
1:A:649:VAL:O	1:A:650:GLU:HB3	1.82	0.77
1:C:505:ARG:NH1	1:C:508:HIS:ND1	2.33	0.77
1:B:625:PHE:CE2	1:C:542:VAL:HG11	2.19	0.77
1:A:683:THR:H	1:A:686:ASN:HD22	1.32	0.77
1:A:613:VAL:HG22	1:A:627:ASP:HB3	1.67	0.77
1:B:745:GLN:O	1:B:746:ALA:HB3	1.85	0.76
1:C:771:VAL:O	1:C:774:PHE:HB2	1.84	0.76
1:A:748:GLU:HG3	1:A:768:TRP:CE2	2.20	0.76
1:C:789:THR:HG22	1:C:790:ASP:H	1.48	0.76
1:C:505:ARG:HG2	1:C:512:ASP:OD1	1.84	0.76
1:B:680:ILE:HG13	1:B:680:ILE:O	1.86	0.75
1:B:740:ARG:HD3	1:B:780:ARG:NH2	2.01	0.75
1:A:594:ILE:HG23	1:A:717:VAL:HG21	1.69	0.75
1:A:663:ASP:HB3	1:A:665:PHE:H	1.51	0.75
1:A:613:VAL:CG2	1:A:627:ASP:HB3	2.16	0.75
1:A:664:LEU:H	1:A:664:LEU:HD12	1.52	0.74
1:A:531:GLN:HE21	1:C:626:ARG:HD2	1.50	0.74
1:A:714:PHE:O	1:A:718:THR:HG22	1.88	0.74
1:A:745:GLN:O	1:A:746:ALA:HB3	1.86	0.74
1:B:653:MET:O	1:B:655:ILE:HG23	1.88	0.73
1:B:740:ARG:HD3	1:B:780:ARG:HH21	1.53	0.73
1:C:649:VAL:N	1:C:684:ASN:HD21	1.85	0.72
1:B:694:TYR:O	1:B:697:TYR:O	2.05	0.72
1:B:829:TYR:HD1	1:B:835:LEU:HA	1.55	0.72
1:C:615:TYR:O	1:C:619:MET:HG3	1.88	0.72
1:B:583:PHE:N	1:B:583:PHE:CD2	2.42	0.72
1:A:766:GLU:O	1:A:770:ILE:HG13	1.90	0.72
1:C:603:ASN:ND2	1:C:794:VAL:HB	2.04	0.72
1:B:505:ARG:HG2	1:B:512:ASP:OD1	1.90	0.72
1:C:661:GLN:HB2	1:C:669:MET:HB2	1.72	0.71
1:C:730:GLU:OE1	1:C:730:GLU:N	2.24	0.71
1:B:670:MET:H	1:B:670:MET:HE3	1.55	0.71
1:B:744:PHE:HA	1:B:747:LEU:HB3	1.73	0.70
1:A:499:TYR:HA	1:A:531:GLN:O	1.91	0.70
1:A:679:LYS:O	1:A:680:ILE:HG22	1.92	0.70
1:C:679:LYS:O	1:C:679:LYS:HE3	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:ILE:HD11	1:C:697:TYR:CD2	2.27	0.69
1:B:613:VAL:CG2	1:B:627:ASP:HB3	2.21	0.69
1:B:722:PRO:O	1:B:723:LEU:HB2	1.93	0.69
1:C:767:PHE:O	1:C:771:VAL:HG23	1.94	0.68
1:B:583:PHE:HD2	1:B:583:PHE:H	0.85	0.68
1:C:611:PRO:HD2	1:C:614:VAL:HG23	1.75	0.68
1:A:749:GLU:O	1:A:751:THR:N	2.27	0.68
1:C:738:GLY:O	1:C:791:ARG:HD3	1.94	0.68
1:B:742:LEU:HD11	1:B:780:ARG:HH12	1.56	0.68
1:B:780:ARG:O	1:B:784:GLN:HG3	1.94	0.67
1:B:613:VAL:O	1:B:617:LYS:HG3	1.94	0.67
1:B:770:ILE:HD13	1:B:836:LYS:HB2	1.74	0.67
1:C:729:PRO:HG2	1:C:730:GLU:OE1	1.94	0.67
1:B:663:ASP:O	1:B:665:PHE:N	2.28	0.67
1:B:829:TYR:CD1	1:B:835:LEU:HA	2.30	0.67
1:C:655:ILE:HG13	1:C:682:ILE:HD12	1.76	0.66
1:B:683:THR:H	1:B:686:ASN:HD22	1.42	0.66
1:C:634:VAL:HG13	1:C:635:LEU:N	2.10	0.66
1:A:559:ILE:HG21	1:A:592:ILE:HD13	1.78	0.66
1:B:740:ARG:CD	1:B:780:ARG:HH21	2.08	0.66
1:B:649:VAL:H	1:B:684:ASN:HD21	1.42	0.66
1:C:757:TYR:CE2	1:C:806:LYS:HA	2.30	0.66
1:A:683:THR:N	1:A:686:ASN:ND2	2.42	0.66
1:A:682:ILE:HA	1:A:686:ASN:HD22	1.61	0.66
1:C:663:ASP:O	1:C:665:PHE:N	2.30	0.65
1:C:655:ILE:CG1	1:C:682:ILE:HD12	2.27	0.65
1:C:787:THR:HG22	1:C:788:GLY:N	2.11	0.65
1:A:813:ARG:HH11	1:A:813:ARG:HB3	1.62	0.65
1:B:711:ARG:HG2	1:B:711:ARG:HH11	1.61	0.65
1:C:574:LYS:O	1:C:575:LEU:HD23	1.97	0.65
1:C:683:THR:C	1:C:685:GLU:H	1.99	0.65
1:A:771:VAL:O	1:A:774:PHE:HB2	1.97	0.64
1:A:531:GLN:NE2	1:C:626:ARG:HD2	2.12	0.64
1:B:564:ILE:HG23	1:B:566:MET:HG3	1.79	0.64
1:A:697:TYR:O	1:A:698:ILE:HB	1.96	0.64
1:C:748:GLU:HG3	1:C:768:TRP:CE2	2.32	0.64
1:B:748:GLU:OE1	1:B:772:HIS:HE1	1.81	0.64
1:A:743:ASP:OD2	1:C:740:ARG:HD3	1.97	0.64
1:A:546:GLY:HA3	1:A:821:PHE:CE2	2.33	0.64
1:A:516:ARG:O	1:A:520:ILE:HG13	1.97	0.64
1:C:744:PHE:HA	1:C:747:LEU:HB3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:PRO:HD2	1:B:614:VAL:HG23	1.80	0.64
1:A:809:PRO:O	1:A:811:THR:HG23	1.98	0.64
1:C:603:ASN:OD1	1:C:793:PRO:HB3	1.98	0.64
1:B:787:THR:HB	1:B:822:ASN:OD1	1.98	0.64
1:A:776:ASP:HB2	1:B:745:GLN:HG3	1.79	0.63
1:C:775:THR:OG1	1:C:778:GLN:HG3	1.98	0.63
1:B:770:ILE:HG22	1:B:774:PHE:CE1	2.33	0.63
1:C:661:GLN:H	1:C:669:MET:H	1.47	0.63
1:B:501:ARG:HA	1:B:533:TYR:O	1.98	0.63
1:C:570:ASP:OD2	1:C:572:SER:HB3	1.98	0.63
1:B:749:GLU:O	1:B:751:THR:N	2.32	0.63
1:A:723:LEU:HD12	1:A:726:LEU:HD12	1.79	0.62
1:B:771:VAL:O	1:B:774:PHE:HB2	1.99	0.62
1:A:711:ARG:HH11	1:A:711:ARG:HG2	1.64	0.62
1:C:704:GLU:HG2	1:C:705:LYS:N	2.14	0.62
1:C:659:ILE:HD13	1:C:673:LEU:HD21	1.81	0.62
1:B:628:LEU:O	1:B:630:ASP:N	2.33	0.62
1:B:757:TYR:CE2	1:B:806:LYS:HA	2.34	0.62
1:B:626:ARG:NH2	1:C:532:LEU:O	2.33	0.62
1:A:680:ILE:O	1:A:680:ILE:HG23	2.00	0.62
1:B:719:ASN:O	1:B:720:GLU:HG3	1.98	0.62
1:C:784:GLN:O	1:C:787:THR:O	2.18	0.62
1:B:600:ILE:HD11	1:B:714:PHE:CZ	2.34	0.62
1:A:774:PHE:O	1:A:779:LYS:HE3	1.99	0.62
1:A:814:LEU:HB3	1:A:842:ALA:HB2	1.82	0.61
1:A:745:GLN:O	1:A:746:ALA:CB	2.48	0.61
1:A:643:LEU:HD21	1:A:691:VAL:HG21	1.82	0.61
1:C:607:ASP:OD2	1:C:609:HIS:HE1	1.84	0.61
1:A:770:ILE:HD13	1:A:836:LYS:HB2	1.82	0.61
1:C:549:LYS:HD3	1:C:820:CYS:HA	1.83	0.61
1:A:767:PHE:CZ	1:A:771:VAL:HG21	2.36	0.61
1:A:543:ASP:OD2	1:C:626:ARG:NH2	2.34	0.61
1:A:618:LEU:HD23	1:A:711:ARG:HD2	1.83	0.60
1:A:518:GLU:O	1:A:521:ALA:HB3	2.01	0.60
1:B:683:THR:N	1:B:686:ASN:HD22	2.00	0.60
1:B:697:TYR:O	1:B:698:ILE:HG12	2.00	0.60
1:C:762:VAL:O	1:C:766:GLU:HG3	2.01	0.60
1:A:516:ARG:HG3	1:A:520:ILE:HD11	1.84	0.60
1:A:502:LEU:HD21	1:A:517:LEU:CD2	2.32	0.60
1:A:505:ARG:HH12	1:A:508:HIS:CG	2.20	0.60
1:B:661:GLN:O	1:B:669:MET:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:TYR:HD2	1:A:694:TYR:O	1.85	0.59
1:B:521:ALA:O	1:B:525:PRO:HG3	2.01	0.59
1:B:747:LEU:O	1:B:751:THR:OG1	2.17	0.59
1:B:595:VAL:HG12	1:B:606:LEU:HD11	1.83	0.59
1:B:821:PHE:HB3	1:B:823:VAL:HG23	1.84	0.59
1:B:748:GLU:HG3	1:B:768:TRP:CE2	2.36	0.59
1:B:760:ASP:CG	1:B:765:ARG:HH21	2.06	0.59
1:C:602:ASN:O	1:C:604:CYS:N	2.33	0.59
1:A:697:TYR:O	1:A:698:ILE:CB	2.50	0.59
1:B:792:ALA:HB2	1:B:797:LEU:HD23	1.83	0.59
1:A:728:ARG:NH2	1:B:603:ASN:HA	2.17	0.59
1:A:746:ALA:HB2	1:C:740:ARG:NH1	2.17	0.59
1:A:504:VAL:O	1:A:536:PHE:HA	2.02	0.59
1:C:532:LEU:HB3	1:C:602:ASN:ND2	2.18	0.58
1:C:655:ILE:CD1	1:C:682:ILE:HD12	2.33	0.58
1:B:626:ARG:HB2	1:C:533:TYR:OH	2.03	0.58
1:B:745:GLN:O	1:B:746:ALA:CB	2.49	0.58
1:A:744:PHE:HA	1:A:747:LEU:HB3	1.84	0.58
1:B:768:TRP:O	1:B:772:HIS:HB2	2.02	0.58
1:C:613:VAL:HG22	1:C:627:ASP:HB3	1.86	0.58
1:B:523:GLU:HG2	1:B:524:ASN:H	1.68	0.58
1:B:504:VAL:O	1:B:536:PHE:HA	2.03	0.58
1:C:649:VAL:O	1:C:650:GLU:CB	2.51	0.58
1:C:603:ASN:HD21	1:C:794:VAL:CB	2.11	0.58
1:B:651:ASP:O	1:B:652:ASP:OD1	2.22	0.58
1:B:697:TYR:O	1:B:698:ILE:CB	2.50	0.58
1:C:814:LEU:CD2	1:C:838:ARG:HD3	2.29	0.58
1:A:618:LEU:HD11	1:A:710:PHE:CE1	2.39	0.58
1:A:507:ASP:O	1:A:508:HIS:ND1	2.37	0.58
1:A:706:GLN:H	1:A:706:GLN:CD	2.06	0.58
1:C:658:GLN:HB2	1:C:677:GLY:O	2.04	0.57
1:A:656:THR:O	1:A:682:ILE:HD11	2.04	0.57
1:A:661:GLN:HG3	1:A:697:TYR:OH	2.04	0.57
1:C:506:ARG:O	1:C:507:ASP:CB	2.47	0.57
1:C:745:GLN:O	1:C:746:ALA:CB	2.48	0.57
1:A:505:ARG:HH22	1:A:508:HIS:CD2	2.23	0.57
1:B:683:THR:HG23	1:B:686:ASN:HD21	1.68	0.57
1:A:683:THR:N	1:A:686:ASN:HD22	2.00	0.57
1:A:725:TYR:O	1:A:726:LEU:HD23	2.03	0.57
1:C:748:GLU:HG3	1:C:768:TRP:CD2	2.40	0.57
1:A:687:ARG:O	1:A:691:VAL:HG23	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ILE:HD11	1:B:832:LYS:HB2	1.86	0.57
1:C:703:VAL:O	1:C:706:GLN:HG2	2.05	0.57
1:A:514:LEU:O	1:A:518:GLU:HB2	2.05	0.57
1:C:757:TYR:O	1:C:761:SER:OG	2.22	0.57
1:A:636:TYR:OH	1:B:544:GLU:HG2	2.05	0.57
1:C:655:ILE:HD12	1:C:682:ILE:HD12	1.87	0.57
1:B:719:ASN:O	1:B:721:SER:N	2.32	0.57
1:A:651:ASP:O	1:A:652:ASP:OD1	2.23	0.57
1:A:663:ASP:HB2	1:A:667:ASN:H	1.70	0.56
1:B:723:LEU:HD23	1:B:732:ILE:CD1	2.35	0.56
1:A:565:GLY:O	1:A:582:SER:HB2	2.04	0.56
1:A:743:ASP:O	1:A:745:GLN:N	2.38	0.56
1:A:775:THR:OG1	1:A:778:GLN:HG3	2.04	0.56
1:B:748:GLU:HA	1:B:768:TRP:CH2	2.40	0.56
1:B:543:ASP:OD1	1:B:547:VAL:HB	2.05	0.56
1:C:723:LEU:HA	1:C:726:LEU:HG	1.88	0.56
1:C:588:GLN:OE1	1:C:588:GLN:N	2.38	0.56
1:B:762:VAL:HG12	1:B:766:GLU:OE1	2.04	0.56
1:C:498:PRO:O	1:C:499:TYR:HB2	2.06	0.56
1:A:505:ARG:NH1	1:A:508:HIS:CG	2.74	0.56
1:C:712:ARG:CZ	1:C:716:MET:HE2	2.36	0.56
1:C:821:PHE:HB2	1:C:823:VAL:HG23	1.87	0.56
1:B:815:PRO:HD3	1:B:829:TYR:OH	2.06	0.56
1:B:667:ASN:N	1:B:667:ASN:HD22	2.05	0.55
1:C:500:LEU:O	1:C:501:ARG:HB2	2.07	0.55
1:C:649:VAL:HG12	1:C:650:GLU:H	1.69	0.55
1:A:719:ASN:O	1:A:720:GLU:HB2	2.06	0.55
1:B:753:TYR:HB2	1:B:757:TYR:O	2.06	0.55
1:A:789:THR:OG1	1:A:790:ASP:N	2.39	0.55
1:C:684:ASN:N	1:C:684:ASN:HD22	2.01	0.55
1:C:697:TYR:O	1:C:698:ILE:CB	2.50	0.55
1:B:697:TYR:O	1:B:698:ILE:HB	2.07	0.55
1:A:679:LYS:O	1:A:680:ILE:CG2	2.54	0.55
1:A:626:ARG:NH2	1:B:543:ASP:OD2	2.39	0.55
1:B:827:PRO:HB2	1:B:829:TYR:CE2	2.42	0.55
1:B:600:ILE:HD11	1:B:714:PHE:HZ	1.71	0.55
1:C:649:VAL:HG23	1:C:684:ASN:HD22	1.69	0.54
1:B:661:GLN:O	1:B:669:MET:HG3	2.07	0.54
1:B:523:GLU:O	1:B:524:ASN:C	2.45	0.54
1:C:613:VAL:CG2	1:C:627:ASP:HB3	2.38	0.54
1:B:556:VAL:HG13	1:B:560:PHE:CD1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:GLN:N	1:A:588:GLN:OE1	2.40	0.54
1:C:728:ARG:NH1	1:C:730:GLU:OE1	2.40	0.54
1:B:723:LEU:HD23	1:B:732:ILE:HD11	1.89	0.54
1:A:523:GLU:O	1:A:524:ASN:C	2.46	0.54
1:C:724:LYS:O	1:C:724:LYS:HD3	2.08	0.54
1:C:704:GLU:O	1:C:705:LYS:HB2	2.07	0.54
1:C:521:ALA:O	1:C:525:PRO:HG3	2.08	0.54
1:C:505:ARG:HH12	1:C:508:HIS:CE1	2.26	0.54
1:C:521:ALA:HB2	1:C:528:LEU:HD11	1.90	0.54
1:A:749:GLU:C	1:A:751:THR:H	2.11	0.54
1:C:683:THR:C	1:C:685:GLU:N	2.61	0.53
1:B:523:GLU:OE1	1:B:524:ASN:O	2.26	0.53
1:A:543:ASP:OD1	1:A:547:VAL:HB	2.07	0.53
1:A:628:LEU:HD23	1:A:699:LEU:HD11	1.89	0.53
1:C:757:TYR:C	1:C:758:THR:HG23	2.29	0.53
1:A:706:GLN:N	1:A:706:GLN:OE1	2.30	0.53
1:A:524:ASN:C	1:A:526:ALA:H	2.12	0.53
1:C:651:ASP:O	1:C:652:ASP:CG	2.47	0.53
1:B:809:PRO:O	1:B:811:THR:HG23	2.08	0.53
1:A:711:ARG:NH1	1:A:711:ARG:HG2	2.23	0.53
1:B:757:TYR:CZ	1:B:806:LYS:HG3	2.43	0.53
1:B:523:GLU:CG	1:B:524:ASN:N	2.72	0.53
1:A:721:SER:HA	1:C:725:TYR:HD1	1.73	0.53
1:C:500:LEU:HG	1:C:527:ASP:O	2.09	0.53
1:B:698:ILE:HG22	1:B:699:LEU:HD12	1.91	0.53
1:B:505:ARG:C	1:B:506:ARG:O	2.46	0.53
1:C:663:ASP:N	1:C:663:ASP:OD1	2.41	0.53
1:A:583:PHE:HD1	1:A:584:GLU:HG2	1.73	0.52
1:B:674:LYS:HD3	1:B:680:ILE:CD1	2.39	0.52
1:C:649:VAL:O	1:C:650:GLU:HB2	2.09	0.52
1:B:776:ASP:O	1:B:780:ARG:HG3	2.09	0.52
1:A:723:LEU:HD22	1:A:723:LEU:N	2.25	0.52
1:C:784:GLN:HG3	1:C:790:ASP:HB3	1.89	0.52
1:B:657:PHE:CG	1:B:680:ILE:HD11	2.44	0.52
1:C:816:THR:OG1	1:C:825:LEU:HD12	2.09	0.52
1:C:649:VAL:HG12	1:C:650:GLU:N	2.24	0.52
1:C:668:PRO:HB2	1:C:670:MET:CE	2.40	0.52
1:C:785:PHE:CG	1:C:843:ILE:HG22	2.44	0.52
1:C:728:ARG:HH11	1:C:729:PRO:HD2	1.71	0.52
1:B:766:GLU:O	1:B:770:ILE:HG13	2.10	0.52
1:C:634:VAL:CG1	1:C:635:LEU:H	2.20	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ASP:O	1:A:508:HIS:CB	2.58	0.52
1:C:809:PRO:O	1:C:811:THR:HG23	2.10	0.52
1:A:720:GLU:C	1:A:722:PRO:CD	2.79	0.52
1:B:669:MET:O	1:B:670:MET:C	2.49	0.52
1:A:523:GLU:OE1	1:A:524:ASN:HB2	2.09	0.52
1:B:830:SER:O	1:B:831:SER:HB2	2.09	0.51
1:C:704:GLU:O	1:C:706:GLN:N	2.44	0.51
1:C:712:ARG:O	1:C:716:MET:HG3	2.09	0.51
1:A:720:GLU:O	1:A:722:PRO:CD	2.52	0.51
1:B:697:TYR:O	1:B:698:ILE:CG1	2.59	0.51
1:A:505:ARG:HH12	1:A:508:HIS:CD2	2.28	0.51
1:C:711:ARG:HG2	1:C:711:ARG:HH11	1.76	0.51
1:A:599:ALA:O	1:A:602:ASN:O	2.28	0.51
1:C:549:LYS:HZ1	1:C:787:THR:HG23	1.75	0.51
1:A:505:ARG:HG2	1:A:512:ASP:OD1	2.11	0.51
1:C:679:LYS:O	1:C:681:PRO:HD3	2.11	0.51
1:A:761:SER:O	1:A:762:VAL:C	2.48	0.51
1:A:837:GLU:OE1	1:A:838:ARG:NH2	2.39	0.51
1:B:662:THR:O	1:B:663:ASP:OD1	2.29	0.51
1:C:671:TYR:CZ	1:C:697:TYR:CE1	2.99	0.51
1:A:507:ASP:O	1:A:508:HIS:HB2	2.11	0.51
1:B:642:LEU:O	1:B:687:ARG:NH1	2.44	0.51
1:B:615:TYR:O	1:B:619:MET:HG3	2.11	0.51
1:B:624:THR:N	1:B:627:ASP:OD2	2.42	0.51
1:C:651:ASP:O	1:C:652:ASP:OD1	2.29	0.51
1:A:555:VAL:HG11	1:A:595:VAL:HG21	1.93	0.51
1:A:607:ASP:OD2	1:A:609:HIS:HE1	1.94	0.51
1:C:748:GLU:HA	1:C:768:TRP:CH2	2.45	0.51
1:B:766:GLU:OE2	1:B:832:LYS:HB3	2.11	0.50
1:A:694:TYR:O	1:A:697:TYR:O	2.29	0.50
1:A:735:LEU:HD11	1:C:727:PHE:CE2	2.46	0.50
1:A:765:ARG:O	1:A:769:GLU:HG3	2.12	0.50
1:B:659:ILE:HD13	1:B:673:LEU:HD21	1.92	0.50
1:B:661:GLN:HB2	1:B:669:MET:HB2	1.93	0.50
1:C:497:ASN:O	1:C:530:LYS:HD3	2.10	0.50
1:B:498:PRO:HG2	1:B:499:TYR:H	1.76	0.50
1:B:748:GLU:OE1	1:B:772:HIS:CE1	2.62	0.50
1:A:748:GLU:HA	1:A:768:TRP:CZ2	2.47	0.50
1:B:645:TYR:CE2	1:B:647:GLY:HA3	2.47	0.50
1:A:677:GLY:O	1:A:679:LYS:O	2.30	0.50
1:C:583:PHE:CE1	1:C:584:GLU:HG3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:LEU:O	1:B:747:LEU:HD13	2.12	0.50
1:C:789:THR:HG22	1:C:790:ASP:N	2.23	0.50
1:C:610:PHE:HB3	1:C:614:VAL:CG2	2.41	0.50
1:C:760:ASP:OD2	1:C:765:ARG:NH2	2.43	0.50
1:A:724:LYS:O	1:A:725:TYR:HB2	2.12	0.50
1:B:783:LEU:O	1:B:787:THR:HG23	2.12	0.50
1:C:532:LEU:HB3	1:C:602:ASN:HD21	1.76	0.50
1:B:770:ILE:HD12	1:B:835:LEU:HD13	1.93	0.49
1:A:655:ILE:HG13	1:A:682:ILE:HD12	1.93	0.49
1:A:549:LYS:HG3	1:A:604:CYS:SG	2.52	0.49
1:C:596:LEU:O	1:C:600:ILE:HG13	2.12	0.49
1:C:570:ASP:O	1:C:572:SER:N	2.45	0.49
1:C:662:THR:HG22	1:C:668:PRO:CA	2.41	0.49
1:B:653:MET:O	1:B:654:MET:C	2.50	0.49
1:A:582:SER:OG	1:A:585:THR:HG21	2.13	0.49
1:B:773:SER:O	1:B:774:PHE:O	2.30	0.49
1:C:567:PHE:HB3	1:C:576:PHE:HB3	1.94	0.49
1:B:776:ASP:HA	1:B:779:LYS:HB2	1.94	0.49
1:C:721:SER:HB2	1:C:722:PRO:HD2	1.94	0.49
1:A:501:ARG:HA	1:A:533:TYR:O	2.12	0.49
1:A:501:ARG:O	1:A:516:ARG:NH1	2.46	0.49
1:B:720:GLU:HG3	1:B:721:SER:H	1.78	0.49
1:C:703:VAL:C	1:C:704:GLU:O	2.51	0.49
1:A:613:VAL:HG21	1:A:627:ASP:HB3	1.94	0.49
1:C:610:PHE:HB3	1:C:614:VAL:HG21	1.94	0.49
1:A:837:GLU:OE2	1:A:838:ARG:HG2	2.12	0.49
1:C:680:ILE:O	1:C:680:ILE:CG1	2.61	0.49
1:A:686:ASN:O	1:A:689:GLU:N	2.46	0.49
1:C:767:PHE:CE1	1:C:771:VAL:HG21	2.48	0.49
1:A:717:VAL:HG12	1:A:717:VAL:O	2.12	0.49
1:A:762:VAL:O	1:A:766:GLU:HG3	2.12	0.49
1:C:698:ILE:H	1:C:702:SER:HB2	1.77	0.48
1:C:757:TYR:CE2	1:C:806:LYS:CA	2.96	0.48
1:B:597:GLY:O	1:B:600:ILE:HB	2.13	0.48
1:A:827:PRO:HD2	1:A:829:TYR:CE1	2.48	0.48
1:C:683:THR:HG23	1:C:686:ASN:ND2	2.28	0.48
1:B:720:GLU:O	1:B:721:SER:C	2.52	0.48
1:A:815:PRO:HD3	1:A:829:TYR:OH	2.13	0.48
1:A:730:GLU:OE1	1:A:730:GLU:N	2.43	0.48
1:A:552:PHE:HD1	1:A:595:VAL:HG13	1.78	0.48
1:C:743:ASP:O	1:C:744:PHE:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:LEU:HD22	1:B:632:HIS:HB2	1.96	0.48
1:B:556:VAL:HG13	1:B:560:PHE:CE1	2.48	0.48
1:A:753:TYR:N	1:A:753:TYR:CD1	2.81	0.48
1:C:555:VAL:HG11	1:C:595:VAL:HG21	1.96	0.48
1:A:744:PHE:H	1:A:797:LEU:HD12	1.79	0.48
1:B:506:ARG:C	1:B:508:HIS:H	2.16	0.48
1:C:787:THR:CG2	1:C:788:GLY:N	2.77	0.48
1:A:800:LEU:O	1:A:801:LYS:C	2.51	0.48
1:B:815:PRO:HB3	1:B:826:LEU:HD23	1.96	0.47
1:B:680:ILE:O	1:B:680:ILE:CG1	2.60	0.47
1:B:775:THR:C	1:B:777:GLU:H	2.18	0.47
1:B:506:ARG:O	1:B:507:ASP:HB2	2.13	0.47
1:A:502:LEU:HD21	1:A:517:LEU:HD21	1.95	0.47
1:B:523:GLU:OE1	1:B:524:ASN:N	2.48	0.47
1:A:736:ILE:HG22	1:A:736:ILE:O	2.13	0.47
1:B:602:ASN:C	1:B:604:CYS:H	2.16	0.47
1:A:684:ASN:HD22	1:A:684:ASN:N	2.12	0.47
1:A:499:TYR:OH	1:C:625:PHE:HB3	2.14	0.47
1:B:500:LEU:HD23	1:B:520:ILE:HD13	1.96	0.47
1:A:552:PHE:CD1	1:A:595:VAL:HG13	2.49	0.47
1:C:543:ASP:OD1	1:C:547:VAL:HB	2.14	0.47
1:B:516:ARG:HG3	1:B:516:ARG:HH11	1.78	0.47
1:C:612:MET:HE3	1:C:730:GLU:HG3	1.96	0.47
1:A:591:LEU:O	1:A:595:VAL:HG23	2.15	0.47
1:B:836:LYS:O	1:B:840:LEU:HG	2.14	0.47
1:B:761:SER:HB2	1:B:764:ILE:HB	1.96	0.47
1:C:730:GLU:O	1:C:734:LEU:HG	2.15	0.47
1:A:583:PHE:CE1	1:A:584:GLU:HG2	2.48	0.47
1:A:533:TYR:HA	1:C:626:ARG:NH2	2.29	0.47
1:A:760:ASP:O	1:A:761:SER:OG	2.30	0.47
1:C:744:PHE:CE1	1:C:779:LYS:HB3	2.50	0.47
1:A:590:THR:O	1:A:594:ILE:HG13	2.15	0.47
1:A:813:ARG:HH11	1:A:813:ARG:CB	2.27	0.47
1:C:719:ASN:ND2	1:C:720:GLU:HG3	2.29	0.47
1:B:679:LYS:O	1:B:681:PRO:HD3	2.15	0.47
1:A:698:ILE:HG22	1:A:699:LEU:CD1	2.45	0.47
1:B:596:LEU:HD12	1:B:606:LEU:CD1	2.44	0.47
1:B:682:ILE:HD13	1:B:690:PHE:CD2	2.48	0.47
1:B:516:ARG:HD2	1:B:516:ARG:HA	1.70	0.47
1:C:674:LYS:HD3	1:C:680:ILE:HD13	1.96	0.47
1:A:763:LEU:HD11	1:A:826:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:GLU:OE2	1:C:832:LYS:HB2	2.15	0.47
1:C:511:ASP:N	1:C:511:ASP:OD2	2.47	0.47
1:C:787:THR:HG22	1:C:788:GLY:H	1.76	0.46
1:C:661:GLN:NE2	1:C:697:TYR:HE2	2.13	0.46
1:A:520:ILE:O	1:A:520:ILE:HG22	2.15	0.46
1:A:711:ARG:O	1:A:715:HIS:HB2	2.15	0.46
1:A:569:TYR:CD1	1:A:576:PHE:CZ	3.03	0.46
1:B:749:GLU:C	1:B:751:THR:H	2.18	0.46
1:C:714:PHE:CZ	1:C:718:THR:HG21	2.50	0.46
1:C:744:PHE:CD1	1:C:779:LYS:HD3	2.51	0.46
1:A:506:ARG:O	1:A:507:ASP:HB2	2.15	0.46
1:B:687:ARG:HA	1:B:690:PHE:HB3	1.98	0.46
1:A:792:ALA:HA	1:A:793:PRO:HD3	1.75	0.46
1:B:670:MET:H	1:B:670:MET:CE	2.25	0.46
1:C:661:GLN:NE2	1:C:697:TYR:CE2	2.84	0.46
1:C:697:TYR:HD1	1:C:701:LYS:HE3	1.81	0.46
1:B:803:ILE:HB	1:B:823:VAL:HG22	1.96	0.46
1:A:643:LEU:HD21	1:A:691:VAL:CG2	2.46	0.46
1:A:762:VAL:HG12	1:A:766:GLU:CD	2.35	0.46
1:A:643:LEU:HA	1:A:687:ARG:HD2	1.98	0.46
1:A:723:LEU:HG	1:A:732:ILE:HD13	1.96	0.46
1:A:740:ARG:NH1	1:A:780:ARG:NH2	2.64	0.46
1:B:657:PHE:CD1	1:B:680:ILE:HG13	2.51	0.46
1:C:741:ASN:HB3	1:C:792:ALA:HB3	1.98	0.46
1:C:744:PHE:CZ	1:C:779:LYS:HB3	2.50	0.46
1:C:762:VAL:HG12	1:C:766:GLU:CD	2.35	0.46
1:C:680:ILE:HG12	1:C:680:ILE:O	2.15	0.46
1:B:594:ILE:O	1:B:598:LEU:HG	2.15	0.46
1:B:667:ASN:N	1:B:667:ASN:ND2	2.62	0.46
1:A:776:ASP:HB2	1:B:745:GLN:HE21	1.81	0.46
1:A:531:GLN:HE22	1:C:626:ARG:HB2	1.81	0.46
1:C:803:ILE:HB	1:C:823:VAL:HG22	1.97	0.46
1:C:838:ARG:HA	1:C:838:ARG:HH11	1.80	0.45
1:C:531:GLN:HE21	1:C:533:TYR:HE1	1.62	0.45
1:C:743:ASP:C	1:C:745:GLN:H	2.18	0.45
1:A:770:ILE:HG13	1:A:832:LYS:HE3	1.99	0.45
1:B:523:GLU:HG2	1:B:524:ASN:N	2.27	0.45
1:C:668:PRO:HB2	1:C:670:MET:HE1	1.98	0.45
1:C:641:ASP:O	1:C:642:LEU:C	2.54	0.45
1:A:583:PHE:O	1:A:584:GLU:HB2	2.16	0.45
1:C:811:THR:OG1	1:C:812:GLU:N	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:757:TYR:HE2	1:C:806:LYS:HA	1.77	0.45
1:C:683:THR:H	1:C:686:ASN:HB2	1.81	0.45
1:C:721:SER:O	1:C:723:LEU:N	2.49	0.45
1:A:741:ASN:O	1:A:742:LEU:HD23	2.17	0.45
1:B:744:PHE:CZ	1:B:779:LYS:HB3	2.52	0.45
1:B:765:ARG:O	1:B:769:GLU:HG3	2.17	0.45
1:A:748:GLU:HA	1:A:768:TRP:CH2	2.52	0.45
1:B:590:THR:O	1:B:594:ILE:HG13	2.16	0.45
1:B:742:LEU:CD1	1:B:776:ASP:HB2	2.47	0.45
1:C:505:ARG:C	1:C:506:ARG:O	2.54	0.45
1:B:606:LEU:HB3	1:B:608:VAL:HG13	1.98	0.45
1:C:763:LEU:HD22	1:C:835:LEU:HD12	1.99	0.45
1:C:549:LYS:NZ	1:C:787:THR:HG23	2.32	0.44
1:C:761:SER:O	1:C:762:VAL:C	2.55	0.44
1:A:589:PHE:CE2	1:A:706:GLN:HB3	2.52	0.44
1:B:771:VAL:O	1:B:779:LYS:HE2	2.17	0.44
1:A:766:GLU:HB3	1:A:832:LYS:HG3	2.00	0.44
1:A:677:GLY:HA2	1:A:680:ILE:CG2	2.47	0.44
1:A:596:LEU:HG	1:A:736:ILE:HD13	1.99	0.44
1:A:755:GLY:O	1:A:806:LYS:HE2	2.17	0.44
1:A:580:PRO:HG3	1:A:703:VAL:CG1	2.48	0.44
1:B:748:GLU:HA	1:B:768:TRP:CZ2	2.53	0.44
1:B:841:LYS:O	1:B:845:TYR:CB	2.65	0.44
1:A:505:ARG:C	1:A:506:ARG:O	2.47	0.44
1:B:764:ILE:O	1:B:767:PHE:HB3	2.16	0.44
1:B:686:ASN:O	1:B:689:GLU:N	2.51	0.44
1:A:722:PRO:C	1:A:724:LYS:H	2.21	0.44
1:C:671:TYR:CE2	1:C:697:TYR:CE1	3.06	0.44
1:C:698:ILE:HG22	1:C:699:LEU:HD13	1.98	0.44
1:B:639:LEU:HD21	1:B:694:TYR:CD1	2.52	0.44
1:C:762:VAL:HG12	1:C:766:GLU:OE1	2.17	0.44
1:B:596:LEU:HD22	1:B:710:PHE:CZ	2.53	0.44
1:B:727:PHE:CZ	1:C:722:PRO:HG2	2.53	0.44
1:A:631:SER:C	1:A:632:HIS:ND1	2.71	0.44
1:B:635:LEU:HD22	1:B:639:LEU:HD11	2.00	0.44
1:B:516:ARG:HG3	1:B:516:ARG:NH1	2.33	0.44
1:C:664:LEU:HD12	1:C:664:LEU:H	1.82	0.44
1:A:718:THR:O	1:A:719:ASN:O	2.36	0.44
1:C:659:ILE:HD11	1:C:697:TYR:CE2	2.52	0.44
1:A:661:GLN:HA	1:A:661:GLN:OE1	2.18	0.44
1:B:782:PHE:HA	1:B:843:ILE:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:LEU:CD1	1:B:780:ARG:HH12	2.27	0.43
1:A:663:ASP:HB2	1:A:667:ASN:N	2.33	0.43
1:A:618:LEU:HD11	1:A:710:PHE:HE1	1.83	0.43
1:C:650:GLU:OE1	1:C:683:THR:HG22	2.18	0.43
1:B:753:TYR:CE1	1:B:759:ARG:HA	2.53	0.43
1:B:523:GLU:O	1:B:525:PRO:N	2.51	0.43
1:B:781:LEU:HD13	1:B:844:THR:HG22	1.99	0.43
1:B:628:LEU:O	1:B:629:GLY:C	2.57	0.43
1:A:549:LYS:HD3	1:A:820:CYS:HA	1.99	0.43
1:B:676:ASN:C	1:B:678:ASP:N	2.71	0.43
1:A:712:ARG:NH2	1:A:716:MET:HE2	2.33	0.43
1:A:655:ILE:CG1	1:A:682:ILE:HD12	2.48	0.43
1:B:674:LYS:O	1:B:675:GLU:C	2.56	0.43
1:B:635:LEU:HD22	1:B:639:LEU:CD1	2.48	0.43
1:A:507:ASP:O	1:A:508:HIS:CG	2.71	0.43
1:A:753:TYR:CE2	1:A:764:ILE:HD12	2.54	0.43
1:A:721:SER:O	1:A:722:PRO:O	2.37	0.43
1:A:532:LEU:HD12	1:A:533:TYR:H	1.84	0.43
1:C:498:PRO:HG2	1:C:499:TYR:CD1	2.54	0.43
1:A:782:PHE:C	1:A:782:PHE:CD1	2.91	0.43
1:B:649:VAL:HG23	1:B:684:ASN:HD21	1.84	0.43
1:A:837:GLU:OE2	1:A:838:ARG:NE	2.48	0.43
1:A:569:TYR:HD1	1:A:576:PHE:CZ	2.37	0.43
1:A:803:ILE:O	1:A:823:VAL:HA	2.19	0.43
1:C:648:ASN:C	1:C:649:VAL:O	2.57	0.43
1:B:824:LEU:HD22	1:B:826:LEU:HG	2.00	0.43
1:C:569:TYR:CZ	1:C:574:LYS:HA	2.54	0.43
1:A:524:ASN:C	1:A:526:ALA:N	2.71	0.43
1:C:662:THR:HG22	1:C:668:PRO:N	2.33	0.43
1:A:714:PHE:CE2	1:A:718:THR:HG21	2.54	0.43
1:B:711:ARG:HG2	1:B:711:ARG:NH1	2.31	0.43
1:C:768:TRP:O	1:C:769:GLU:C	2.56	0.43
1:B:761:SER:HB2	1:B:764:ILE:HG12	2.01	0.43
1:B:588:GLN:OE1	1:B:588:GLN:N	2.52	0.43
1:C:792:ALA:HA	1:C:793:PRO:HD3	1.77	0.43
1:B:649:VAL:O	1:B:650:GLU:CB	2.61	0.43
1:C:570:ASP:O	1:C:571:GLU:C	2.55	0.43
1:A:708:LYS:O	1:A:712:ARG:HG3	2.18	0.43
1:C:813:ARG:HB3	1:C:813:ARG:HH11	1.84	0.43
1:B:511:ASP:N	1:B:511:ASP:OD1	2.49	0.43
1:C:681:PRO:O	1:C:686:ASN:ND2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:THR:O	1:B:627:ASP:N	2.52	0.43
1:B:722:PRO:HB3	1:B:725:TYR:HD2	1.83	0.43
1:B:648:ASN:O	1:B:652:ASP:HB2	2.19	0.43
1:A:722:PRO:HG2	1:A:724:LYS:HB2	2.01	0.42
1:C:715:HIS:O	1:C:719:ASN:HB2	2.19	0.42
1:C:807:ASN:O	1:C:813:ARG:NH2	2.45	0.42
1:B:743:ASP:O	1:B:745:GLN:N	2.43	0.42
1:C:761:SER:HB2	1:C:764:ILE:HG12	2.01	0.42
1:C:566:MET:HE3	1:C:589:PHE:CD2	2.54	0.42
1:B:670:MET:N	1:B:670:MET:CE	2.82	0.42
1:C:669:MET:O	1:C:671:TYR:N	2.52	0.42
1:B:775:THR:HG1	1:B:778:GLN:HG3	1.79	0.42
1:B:600:ILE:HD13	1:B:723:LEU:HD11	2.00	0.42
1:C:721:SER:C	1:C:723:LEU:H	2.22	0.42
1:A:500:LEU:HD23	1:A:500:LEU:C	2.39	0.42
1:C:674:LYS:HD3	1:C:680:ILE:CD1	2.49	0.42
1:B:598:LEU:HD23	1:B:717:VAL:HG11	2.01	0.42
1:B:612:MET:HE1	1:B:733:GLU:OE2	2.19	0.42
1:B:611:PRO:HD2	1:B:614:VAL:CG2	2.46	0.42
1:C:516:ARG:CB	1:C:516:ARG:NH1	2.72	0.42
1:A:664:LEU:HD13	1:A:665:PHE:CG	2.54	0.42
1:A:532:LEU:O	1:C:626:ARG:NH2	2.53	0.42
1:C:655:ILE:HG13	1:C:682:ILE:HB	2.02	0.42
1:B:648:ASN:OD1	1:B:651:ASP:OD1	2.37	0.42
1:C:532:LEU:N	1:C:602:ASN:HD21	2.09	0.42
1:A:686:ASN:O	1:A:687:ARG:C	2.58	0.42
1:A:594:ILE:HG23	1:A:717:VAL:CG2	2.44	0.42
1:A:559:ILE:HG21	1:A:592:ILE:CD1	2.46	0.42
1:B:523:GLU:OE1	1:B:523:GLU:C	2.58	0.42
1:A:655:ILE:HG13	1:A:682:ILE:HB	2.02	0.42
1:A:721:SER:HA	1:C:725:TYR:CD1	2.53	0.42
1:A:499:TYR:HB3	1:A:533:TYR:HB2	2.02	0.42
1:A:705:LYS:HD3	1:A:705:LYS:HA	1.82	0.42
1:C:566:MET:HE3	1:C:589:PHE:CE2	2.55	0.42
1:B:838:ARG:HA	1:B:838:ARG:NE	2.34	0.42
1:C:602:ASN:C	1:C:604:CYS:H	2.22	0.41
1:C:743:ASP:HB3	1:C:745:GLN:O	2.20	0.41
1:C:711:ARG:HG2	1:C:711:ARG:NH1	2.33	0.41
1:B:498:PRO:HG2	1:B:499:TYR:N	2.34	0.41
1:A:826:LEU:CD2	1:A:829:TYR:HE1	2.32	0.41
1:A:730:GLU:O	1:A:734:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ILE:CD1	1:B:723:LEU:HD11	2.50	0.41
1:C:662:THR:HG22	1:C:668:PRO:HA	2.03	0.41
1:C:708:LYS:HB3	1:C:708:LYS:NZ	2.35	0.41
1:A:649:VAL:O	1:A:650:GLU:CB	2.58	0.41
1:C:599:ALA:O	1:C:602:ASN:O	2.38	0.41
1:B:720:GLU:HG3	1:B:721:SER:N	2.35	0.41
1:B:608:VAL:HG23	1:B:608:VAL:O	2.20	0.41
1:A:548:SER:O	1:A:551:PHE:HB3	2.20	0.41
1:A:505:ARG:NH2	1:A:508:HIS:CD2	2.88	0.41
1:A:648:ASN:HB3	1:A:651:ASP:HB2	2.02	0.41
1:B:659:ILE:CD1	1:B:673:LEU:HD21	2.50	0.41
1:A:615:TYR:O	1:A:619:MET:HG3	2.19	0.41
1:C:684:ASN:N	1:C:684:ASN:ND2	2.68	0.41
1:B:663:ASP:OD1	1:B:669:MET:SD	2.78	0.41
1:C:505:ARG:O	1:C:506:ARG:C	2.57	0.41
1:B:628:LEU:HD23	1:B:699:LEU:HD11	2.01	0.41
1:A:505:ARG:HD3	1:A:537:GLU:OE1	2.20	0.41
1:B:817:SER:HB2	1:B:823:VAL:O	2.20	0.41
1:B:687:ARG:O	1:B:691:VAL:HG23	2.19	0.41
1:B:728:ARG:O	1:B:731:GLU:HB2	2.21	0.41
1:B:800:LEU:O	1:B:801:LYS:C	2.58	0.41
1:B:775:THR:HG23	1:B:778:GLN:OE1	2.20	0.41
1:A:768:TRP:HA	1:A:768:TRP:CE3	2.55	0.41
1:A:770:ILE:HD11	1:A:832:LYS:HG3	2.02	0.41
1:A:748:GLU:HG3	1:A:768:TRP:CD2	2.56	0.41
1:C:712:ARG:NH1	1:C:716:MET:CE	2.83	0.41
1:B:643:LEU:HD21	1:B:691:VAL:HG21	2.03	0.41
1:C:497:ASN:CB	1:C:498:PRO:CD	2.99	0.41
1:A:757:TYR:CE2	1:A:806:LYS:HA	2.56	0.41
1:C:683:THR:N	1:C:686:ASN:HD22	2.19	0.41
1:A:643:LEU:CD2	1:A:691:VAL:HG21	2.48	0.41
1:A:740:ARG:NH1	1:B:743:ASP:OD2	2.53	0.41
1:A:837:GLU:CD	1:A:838:ARG:HE	2.24	0.41
1:B:624:THR:O	1:B:627:ASP:HB2	2.21	0.41
1:A:677:GLY:O	1:A:678:ASP:C	2.59	0.41
1:B:500:LEU:O	1:B:501:ARG:CB	2.69	0.40
1:C:813:ARG:HH11	1:C:813:ARG:CB	2.34	0.40
1:C:703:VAL:O	1:C:704:GLU:O	2.39	0.40
1:C:821:PHE:CB	1:C:823:VAL:HG23	2.52	0.40
1:C:617:LYS:HA	1:C:621:LYS:O	2.20	0.40
1:A:737:CYS:O	1:A:791:ARG:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:ASN:O	1:C:678:ASP:N	2.50	0.40
1:B:649:VAL:HG23	1:B:684:ASN:ND2	2.36	0.40
1:A:744:PHE:O	1:A:748:GLU:N	2.51	0.40
1:C:723:LEU:HG	1:C:726:LEU:HD12	2.04	0.40
1:B:514:LEU:HD21	1:B:591:LEU:HB2	2.03	0.40
1:C:635:LEU:HD11	1:C:694:TYR:CE2	2.57	0.40
1:C:698:ILE:HG22	1:C:699:LEU:CD1	2.52	0.40
1:B:830:SER:O	1:B:831:SER:CB	2.69	0.40
1:B:761:SER:HB2	1:B:764:ILE:CG1	2.52	0.40
1:B:748:GLU:C	1:B:749:GLU:O	2.56	0.40
1:B:658:GLN:CD	1:B:670:MET:HB3	2.42	0.40
1:B:684:ASN:N	1:B:684:ASN:HD22	2.19	0.40
1:B:505:ARG:NH1	1:B:508:HIS:CG	2.89	0.40
1:B:723:LEU:HA	1:B:726:LEU:HG	2.04	0.40
1:C:770:ILE:HG13	1:C:832:LYS:HE3	2.04	0.40
1:C:548:SER:O	1:C:551: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	348/358 (97%)	279 (80%)	50 (14%)	19 (6%)	2 6
1	B	348/358 (97%)	282 (81%)	47 (14%)	19 (6%)	2 6
1	C	348/358 (97%)	285 (82%)	47 (14%)	16 (5%)	3 9
All	All	1044/1074 (97%)	846 (81%)	144 (14%)	54 (5%)	2 7

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	663	ASP
1	A	698	ILE
1	A	719	ASN
1	A	722	PRO
1	A	750	THR
1	B	650	GLU
1	B	664	LEU
1	B	670	MET
1	B	675	GLU
1	B	698	ILE
1	B	723	LEU
1	B	750	THR
1	B	774	PHE
1	C	652	ASP
1	C	664	LEU
1	C	675	GLU
1	A	527	ASP
1	A	650	GLU
1	A	761	SER
1	B	629	GLY
1	B	654	MET
1	B	687	ARG
1	B	720	GLU
1	B	831	SER
1	C	571	GLU
1	C	670	MET
1	C	704	GLU
1	A	499	TYR
1	A	675	GLU
1	A	687	ARG
1	A	744	PHE
1	B	652	ASP
1	B	829	TYR
1	C	507	ASP
1	C	603	ASN
1	C	650	GLU
1	B	506	ARG
1	B	773	SER
1	C	705	LYS
1	C	758	THR
1	A	612	MET
1	A	721	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	704	GLU
1	A	746	ALA
1	C	499	TYR
1	C	509	ILE
1	C	649	VAL
1	A	524	ASN
1	A	677	GLY
1	A	762	VAL
1	C	698	ILE
1	B	524	ASN
1	C	722	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	317/323 (98%)	295 (93%)	22 (7%)	19 48
1	B	317/323 (98%)	295 (93%)	22 (7%)	19 48
1	C	317/323 (98%)	296 (93%)	21 (7%)	21 51
All	All	951/969 (98%)	886 (93%)	65 (7%)	20 49

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	LEU
1	A	523	GLU
1	A	592	ILE
1	A	616	ARG
1	A	635	LEU
1	A	642	LEU
1	A	664	LEU
1	A	668	PRO
1	A	676	ASN
1	A	678	ASP
1	A	684	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	694	TYR
1	A	706	GLN
1	A	741	ASN
1	A	757	TYR
1	A	774	PHE
1	A	789	THR
1	A	812	GLU
1	A	813	ARG
1	A	824	LEU
1	A	826	LEU
1	A	835	LEU
1	B	501	ARG
1	B	511	ASP
1	B	516	ARG
1	B	523	GLU
1	B	583	PHE
1	B	592	ILE
1	B	602	ASN
1	B	603	ASN
1	B	635	LEU
1	B	642	LEU
1	B	651	ASP
1	B	676	ASN
1	B	694	TYR
1	B	704	GLU
1	B	706	GLN
1	B	720	GLU
1	B	743	ASP
1	B	777	GLU
1	B	787	THR
1	B	824	LEU
1	B	835	LEU
1	B	839	LEU
1	C	502	LEU
1	C	511	ASP
1	C	514	LEU
1	C	516	ARG
1	C	635	LEU
1	C	642	LEU
1	C	670	MET
1	C	676	ASN
1	C	679	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	680	ILE
1	C	694	TYR
1	C	706	GLN
1	C	728	ARG
1	C	743	ASP
1	C	758	THR
1	C	774	PHE
1	C	789	THR
1	C	824	LEU
1	C	826	LEU
1	C	835	LEU
1	C	839	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	HIS
1	A	531	GLN
1	A	609	HIS
1	A	667	ASN
1	A	684	ASN
1	A	686	ASN
1	A	772	HIS
1	B	524	ASN
1	B	667	ASN
1	B	684	ASN
1	B	686	ASN
1	B	772	HIS
1	C	531	GLN
1	C	602	ASN
1	C	609	HIS
1	C	661	GLN
1	C	667	ASN
1	C	684	ASN
1	C	686	ASN
1	C	706	GLN
1	C	715	HIS
1	C	719	ASN
1	C	772	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	350/358 (97%)	-0.16	6 (1%) 73 63	28, 49, 76, 100	0
1	B	350/358 (97%)	0.02	15 (4%) 39 27	24, 51, 89, 124	0
1	C	350/358 (97%)	-0.14	12 (3%) 49 36	20, 43, 80, 127	0
All	All	1050/1074 (97%)	-0.10	33 (3%) 52 40	20, 47, 85, 127	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	664	LEU	9.5
1	C	665	PHE	7.9
1	B	665	PHE	6.4
1	B	667	ASN	6.4
1	B	845	TYR	5.2
1	A	721	SER	4.8
1	B	846	ALA	4.4
1	C	669	MET	4.2
1	B	664	LEU	4.1
1	A	522	MET	4.0
1	C	845	TYR	3.7
1	B	720	GLU	3.5
1	C	667	ASN	3.5
1	B	666	GLY	3.1
1	C	651	ASP	3.1
1	C	666	GLY	3.1
1	B	759	ARG	3.0
1	B	669	MET	2.9
1	B	679	LYS	2.9
1	C	671	TYR	2.9
1	A	584	GLU	2.7
1	A	524	ASN	2.7
1	C	663	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	814	LEU	2.3
1	B	758	THR	2.3
1	A	525	PRO	2.2
1	C	846	ALA	2.1
1	B	583	PHE	2.1
1	B	651	ASP	2.1
1	A	679	LYS	2.0
1	C	782	PHE	2.0
1	B	841	LYS	2.0
1	C	662	THR	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 carbohydrates 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.