Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:37 PM GMT

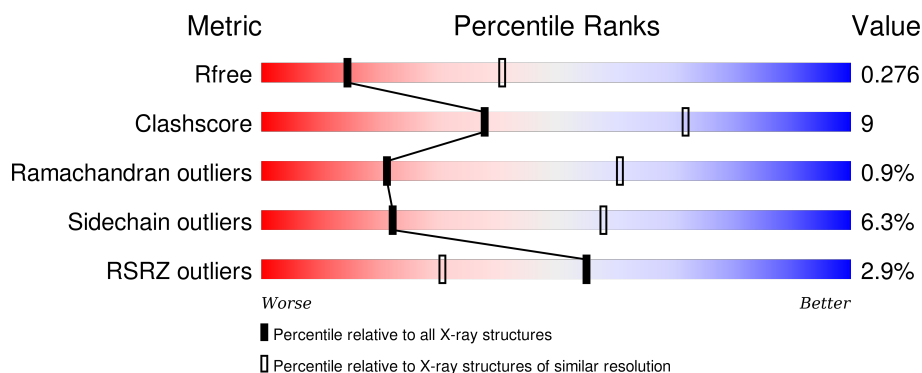|		
PDB ID	:	5CSK
Title	:	Crystal structure of yeast acetyl-CoA carboxylase, unbiotinylated
Authors	:	Wei, J.; Tong, L.
Deposited on	:	2015-07-23
Resolution	:	3.10 Å(reported)

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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 3.10 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		9
Ramachandran outliers		0.9%
Sidechain outliers		6.3%
RSRZ outliers		2.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	2218	2% / 69% / 20% / • / 10%
1	B	2218	4% / 68% / 20% / • / 9%

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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 31806 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1996	Total	C	N	O	S	0	0	0
			15828	10063	2733	2980	52			
1	B	2017	Total	C	N	O	S	0	0	0
			15978	10159	2758	3009	52			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	HIS	-	expression tag	UNP Q00955
A	2235	HIS	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
B	2234	HIS	-	expression tag	UNP Q00955
B	2235	HIS	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955

3 Residue-property plots ⓘ

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: Acetyl-CoA carboxylase
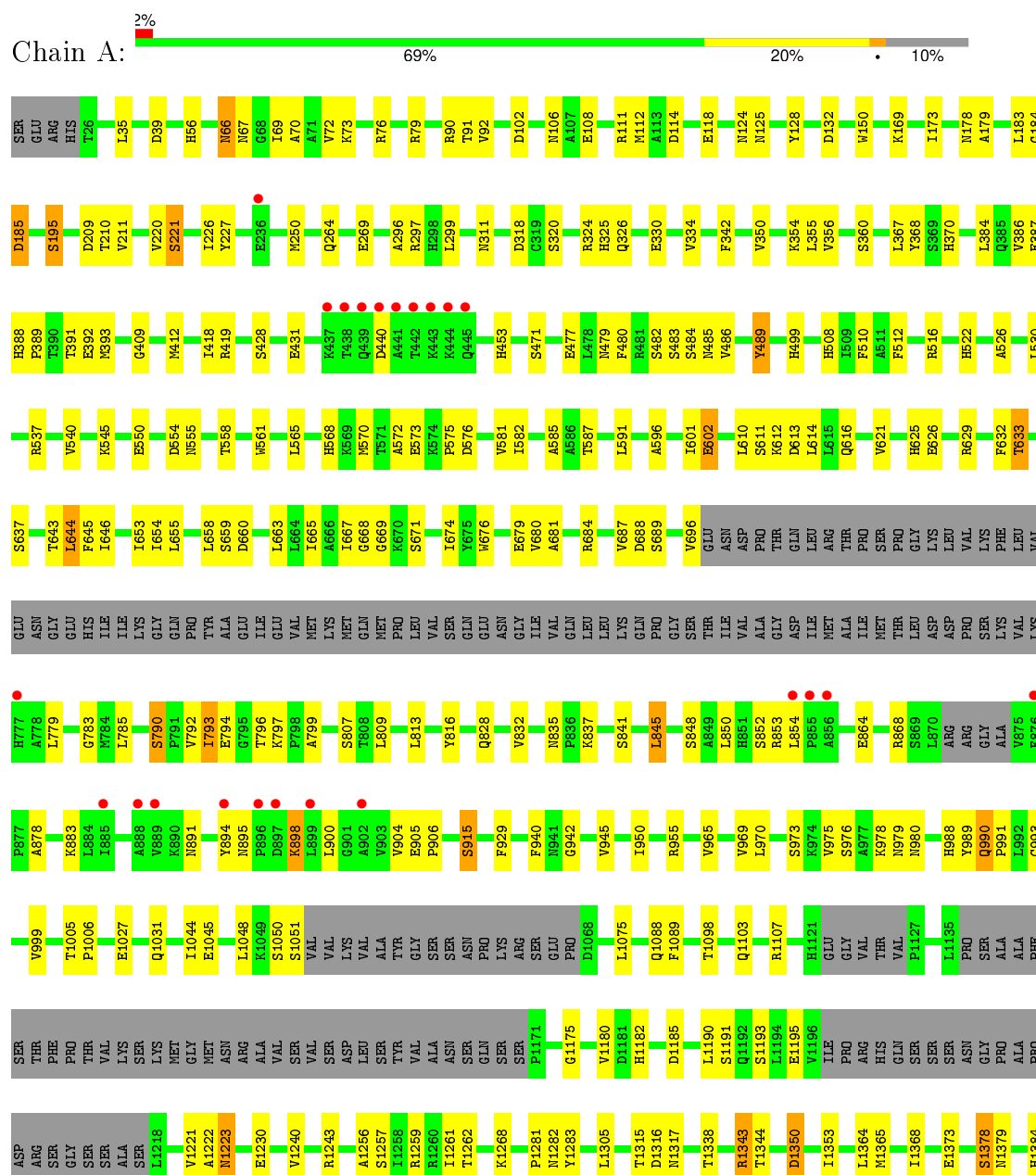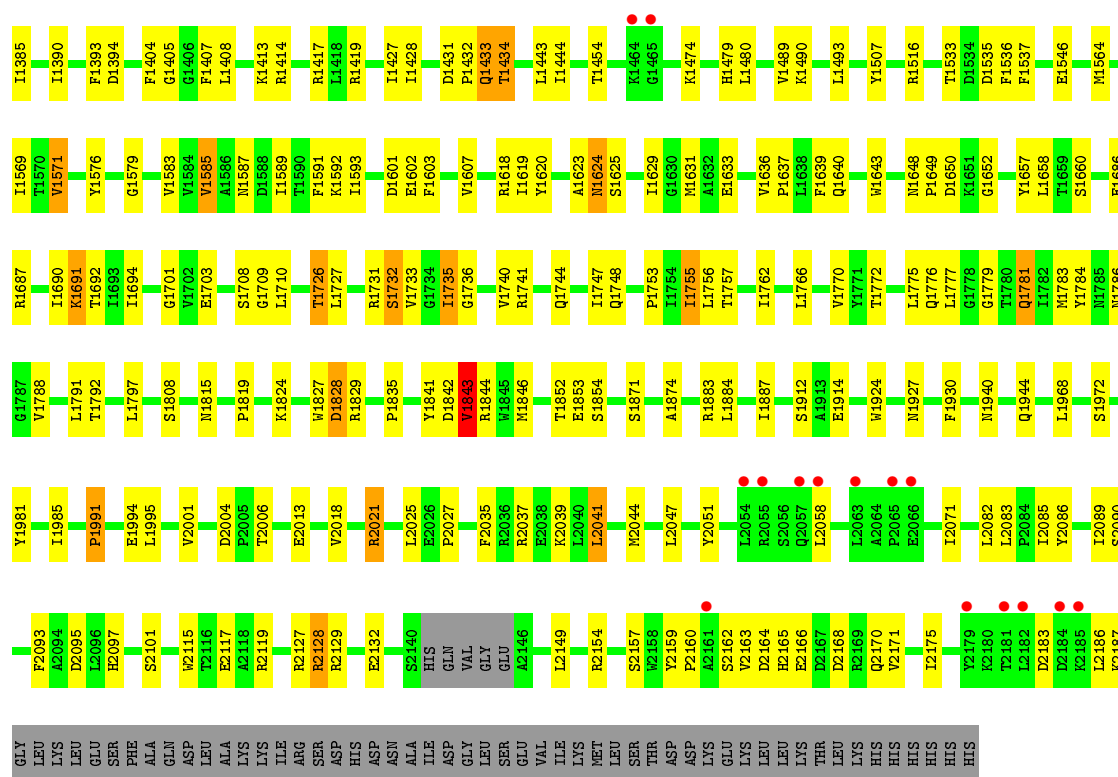
• **Molecule 1: Acetyl-CoA carboxylase**
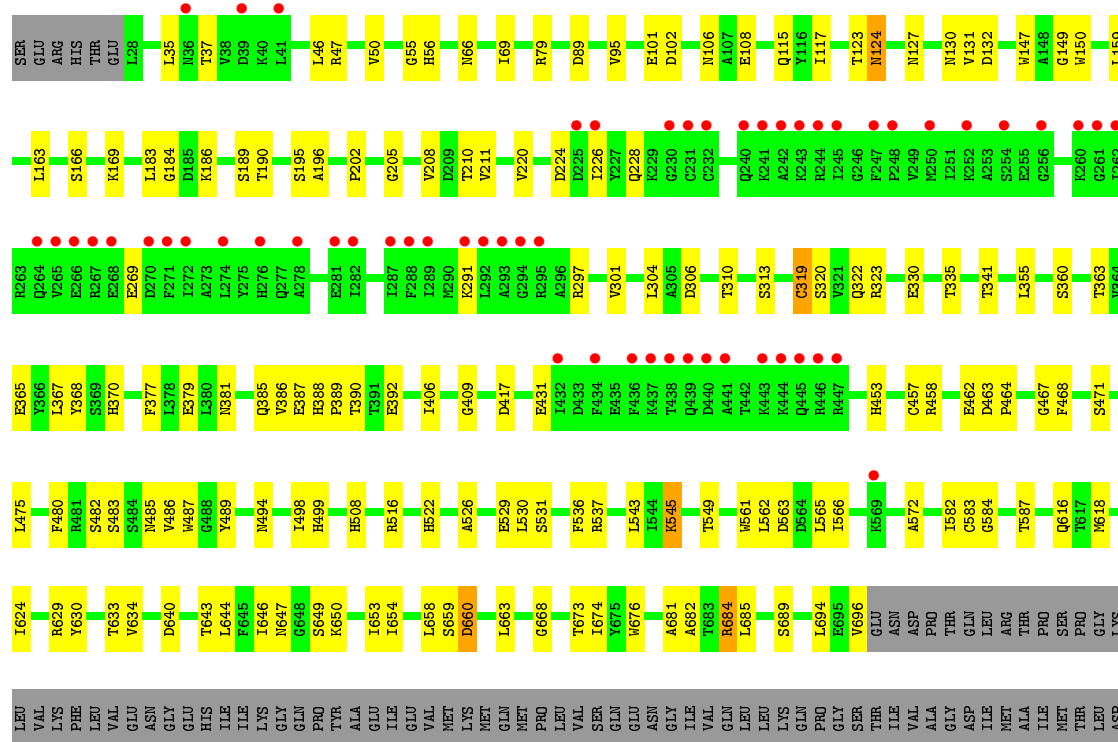
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.88Å 159.88Å 615.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.10 49.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.47-3.10) 93.1 (49.42-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.281 0.218 , 0.276	Depositor DCC
R_{free} test set	6821 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	85.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 135996 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31806	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.56	0/16156	0.76	4/21869 (0.0%)
1	B	0.55	0/16306	0.76	10/22069 (0.0%)
All	All	0.56	0/32462	0.76	14/43938 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1419	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	660	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	1580	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	1571	VAL	CB-CA-C	-5.86	100.27	111.40
1	B	1108	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	660	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	1419	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	1497	ARG	CG-CD-NE	-5.36	100.54	111.80
1	B	2120	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	1343	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	1601	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	1431	ASP	C-N-CD	5.15	139.22	128.40
1	B	1585	VAL	CB-CA-C	-5.11	101.69	111.40
1	A	1571	VAL	CB-CA-C	-5.08	101.75	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15828	0	15783	289	1
1	B	15978	0	15941	323	0
All	All	31806	0	31724	582	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 9.

All (582) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:ILE:H	1:A:1735:ILE:HD13	1.19	1.07
1:B:1040:ARG:NH1	1:B:1081:VAL:O	2.02	0.92
1:B:941:ASN:HD21	1:B:1013:LEU:HA	1.31	0.92
1:A:1243:ARG:NH1	1:A:1283:TYR:O	2.02	0.91
1:A:587:THR:HG22	1:A:663:LEU:HD12	1.53	0.91
1:B:323:ARG:CZ	1:B:468:PHE:CE2	2.54	0.90
1:B:1135:LEU:HB3	1:B:1136:PRO:HD2	1.51	0.90
1:A:1431:ASP:OD2	1:A:1434:THR:OG1	1.93	0.86
1:A:220:VAL:HG21	1:A:355:LEU:HG	1.60	0.83
1:B:587:THR:HG22	1:B:663:LEU:HD12	1.61	0.82
1:A:853:ARG:NH2	1:B:123:THR:OG1	2.12	0.81
1:A:945:VAL:HG11	1:A:950:ILE:HD11	1.63	0.79
1:A:296:ALA:HB3	1:A:367:LEU:HD11	1.65	0.78
1:A:1643:TRP:CE3	1:A:1649:PRO:HB2	2.18	0.78
1:A:2163:VAL:HA	1:A:2170:GLN:NE2	1.98	0.78
1:B:467:GLY:O	1:B:468:PHE:CD2	2.37	0.77
1:B:1766:LEU:HD12	1:B:1770:VAL:HG11	1.66	0.77
1:A:970:LEU:O	1:A:973:SER:OG	2.02	0.77
1:B:1317:ASN:HB3	1:B:1371:ASN:HD21	1.48	0.76
1:B:323:ARG:CZ	1:B:566:ILE:HG12	2.14	0.76
1:B:563:ASP:HA	1:B:566:ILE:HD12	1.68	0.76
1:A:69:ILE:HG23	1:A:489:TYR:CE1	2.21	0.74
1:A:1841:TYR:CE1	1:A:1846:MET:HE3	2.22	0.74
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.68	0.73
1:B:822:MET:SD	1:B:981:LEU:HA	2.30	0.71
1:A:2004:ASP:OD2	1:A:2006:THR:HG22	1.88	0.71
1:B:124:ASN:HA	1:B:127:ASN:OD1	1.90	0.71
1:B:365:GLU:OE2	1:B:381:ASN:OD1	2.08	0.71
1:A:106:ASN:HD21	1:B:658:LEU:HB3	1.56	0.71
1:B:1084:ASP:HB3	1:B:1273:PRO:HD3	1.72	0.70
1:B:1444:ILE:HG23	1:B:1454:THR:HG22	1.73	0.70
1:A:545:LYS:HD2	1:A:572:ALA:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:ILE:H	1:A:1735:ILE:CD1	1.99	0.70
1:A:1841:TYR:CE1	1:A:1846:MET:CE	2.74	0.70
1:B:319:CYS:SG	1:B:330:GLU:CD	2.70	0.69
1:A:330:GLU:OE2	1:A:387:GLU:HB3	1.93	0.69
1:A:1735:ILE:N	1:A:1735:ILE:HD13	2.01	0.69
1:A:106:ASN:OD1	1:A:111:ARG:NH1	2.25	0.69
1:A:611:SER:OG	1:A:612:LYS:N	2.25	0.69
1:B:1135:LEU:HB3	1:B:1136:PRO:CD	2.23	0.69
1:A:483:SER:HB3	1:A:486:VAL:HB	1.75	0.69
1:A:1835:PRO:HG3	1:A:1846:MET:HE1	1.76	0.68
1:B:1301:GLU:OE2	1:B:1441:ARG:NH2	2.23	0.67
1:B:2189:LEU:O	1:B:2193:SER:OG	2.10	0.67
1:B:1350:ASP:N	1:B:1350:ASP:OD1	2.27	0.67
1:B:2163:VAL:HA	1:B:2170:GLN:OE1	1.95	0.67
1:B:323:ARG:NH2	1:B:468:PHE:CE2	2.63	0.67
1:B:1653:PHE:H	1:B:1653:PHE:HD2	1.43	0.66
1:A:453:HIS:CD2	1:A:516:ARG:HA	2.30	0.66
1:A:2021:ARG:HD3	1:A:2095:ASP:OD2	1.96	0.65
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.32	0.65
1:B:1317:ASN:HB3	1:B:1371:ASN:ND2	2.11	0.65
1:A:1835:PRO:HG3	1:A:1846:MET:CE	2.26	0.65
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.32	0.65
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.44	0.64
1:A:965:VAL:O	1:A:969:VAL:HG23	1.97	0.64
1:A:108:GLU:O	1:A:112:MET:HG3	1.97	0.64
1:B:1081:VAL:HG13	1:B:1084:ASP:OD1	1.98	0.64
1:B:453:HIS:CD2	1:B:516:ARG:HA	2.33	0.64
1:B:1078:SER:O	1:B:1108:ARG:NH2	2.31	0.63
1:A:1835:PRO:CG	1:A:1846:MET:HE1	2.28	0.63
1:A:1533:THR:OG1	1:A:1535:ASP:OD2	2.17	0.63
1:A:828:GLN:O	1:A:832:VAL:HG23	1.98	0.63
1:B:323:ARG:NH2	1:B:468:PHE:HE2	1.97	0.63
1:B:319:CYS:SG	1:B:330:GLU:OE2	2.57	0.63
1:A:1005:THR:HB	1:A:1006:PRO:HD3	1.81	0.63
1:B:387:GLU:OE2	1:B:458:ARG:NH2	2.32	0.63
1:B:1770:VAL:HG13	1:B:1771:TYR:CD1	2.33	0.63
1:A:1223:ASN:HB3	1:A:1262:THR:HB	1.79	0.63
1:B:955:ARG:NH1	1:B:1914:GLU:OE1	2.32	0.63
1:A:1593:ILE:HG22	1:A:1625:SER:OG	1.98	0.62
1:A:1972:SER:HB3	1:B:1742:LEU:HD13	1.79	0.62
1:A:485:ASN:HB3	1:A:512:PHE:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLU:HB3	1:B:499:HIS:CG	2.34	0.62
1:A:485:ASN:OD1	1:A:522:HIS:CD2	2.53	0.62
1:A:484:SER:OG	1:A:485:ASN:OD1	2.17	0.62
1:A:69:ILE:CG2	1:A:489:TYR:CE1	2.82	0.62
1:B:1222:ALA:O	1:B:1261:ILE:HA	1.99	0.62
1:A:368:TYR:OH	1:A:370:HIS:HD2	1.83	0.61
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.82	0.61
1:B:1730:CYS:HA	1:B:1752:GLN:OE1	2.01	0.61
1:A:324:ARG:O	1:A:325:HIS:HB2	1.99	0.61
1:A:211:VAL:HG13	1:A:220:VAL:HG13	1.83	0.61
1:A:102:ASP:OD1	1:A:499:HIS:NE2	2.32	0.61
1:B:900:LEU:O	1:B:904:VAL:HG22	2.01	0.60
1:A:2041:LEU:HD11	1:A:2051:TYR:OH	2.01	0.60
1:B:2174:TRP:CE3	1:B:2174:TRP:O	2.53	0.60
1:B:224:ASP:O	1:B:228:GLN:HG2	2.00	0.60
1:A:945:VAL:CG1	1:A:950:ILE:HD11	2.31	0.60
1:B:1344:THR:HG21	1:B:1393:PHE:HZ	1.67	0.60
1:A:486:VAL:HG11	1:A:526:ALA:CB	2.32	0.60
1:A:132:ASP:HB2	1:B:848:SER:OG	2.02	0.59
1:B:2174:TRP:CD2	1:B:2174:TRP:O	2.55	0.59
1:B:905:GLU:HB3	1:B:906:PRO:HD3	1.85	0.59
1:B:1657:TYR:HB2	1:B:1688:PHE:O	2.02	0.59
1:A:568:HIS:O	1:A:570:MET:N	2.35	0.59
1:B:101:GLU:HB3	1:B:499:HIS:CD2	2.37	0.59
1:A:2041:LEU:CD1	1:A:2051:TYR:OH	2.50	0.59
1:A:900:LEU:O	1:A:904:VAL:HG22	2.02	0.59
1:A:1564:MET:CE	1:A:1585:VAL:HG12	2.33	0.58
1:B:150:TRP:CE2	1:B:386:VAL:HB	2.38	0.58
1:A:1378:SER:HB3	1:A:1379:ASN:OD1	2.03	0.58
1:A:679:GLU:OE2	1:A:684:ARG:NH1	2.37	0.58
1:B:583:CYS:SG	1:B:674:ILE:HD11	2.43	0.58
1:A:1088:GLN:HG3	1:A:1268:LYS:HD3	1.86	0.58
1:B:654:ILE:HD12	1:B:792:VAL:HG23	1.86	0.58
1:A:2160:PRO:HB2	1:A:2162:SER:OG	2.03	0.58
1:B:1748:GLN:NE2	1:B:1789:SER:OG	2.37	0.58
1:B:1338:THR:HG21	1:B:1368:ILE:HG23	1.86	0.57
1:B:1466:GLU:O	1:B:1468:VAL:HG23	2.03	0.57
1:A:79:ARG:NH2	1:A:114:ASP:OD2	2.38	0.57
1:A:1784:TYR:HH	1:A:1871:SER:HG	1.48	0.57
1:B:1843:VAL:HG21	1:B:1878:VAL:HG21	1.85	0.57
1:B:1593:ILE:CG2	1:B:1731:ARG:HH21	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ASN:HB2	1:B:522:HIS:HD2	1.70	0.56
1:A:1182:HIS:HE1	1:A:1230:GLU:O	1.87	0.56
1:A:1489:VAL:HG12	1:A:1490:LYS:H	1.70	0.56
1:B:1580:ARG:NH2	1:B:1810:VAL:O	2.34	0.56
1:B:658:LEU:O	1:B:660:ASP:O	2.24	0.56
1:A:125:ASN:OD1	1:B:853:ARG:NH2	2.38	0.56
1:A:790:SER:OG	1:A:792:VAL:O	2.22	0.56
1:B:387:GLU:O	1:B:390:THR:OG1	2.18	0.56
1:A:1827:TRP:O	1:A:1829:ARG:N	2.38	0.56
1:B:561:TRP:CE2	1:B:565:LEU:HD11	2.40	0.56
1:B:799:ALA:O	1:B:803:LYS:HG3	2.06	0.55
1:A:848:SER:OG	1:B:132:ASP:HB2	2.06	0.55
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.88	0.55
1:A:297:ARG:NH2	1:A:555:ASN:O	2.40	0.55
1:B:2115:TRP:O	1:B:2118:ALA:N	2.36	0.55
1:B:205:GLY:O	1:B:208:VAL:HG23	2.06	0.55
1:B:1127:PRO:O	1:B:1128:ILE:HG13	2.06	0.55
1:A:1694:ILE:HA	1:B:2102:ARG:HD3	1.88	0.55
1:B:463:ASP:CG	1:B:537:ARG:HD2	2.27	0.55
1:B:1766:LEU:HD12	1:B:1770:VAL:CG1	2.35	0.55
1:B:1770:VAL:HG13	1:B:1771:TYR:N	2.20	0.55
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.10	0.55
1:B:1406:GLY:HA2	1:B:1409:GLU:HG3	1.89	0.55
1:B:654:ILE:HD12	1:B:792:VAL:CG2	2.36	0.55
1:A:1658:LEU:HD13	1:A:1690:ILE:HD11	1.88	0.55
1:B:1305:LEU:HB3	1:B:1310:ILE:HD11	1.89	0.55
1:B:1406:GLY:HA2	1:B:1409:GLU:CG	2.36	0.55
1:A:637:SER:HA	1:A:816:TYR:HB3	1.89	0.55
1:B:1829:ARG:HB2	1:B:1830:PRO:HD2	1.89	0.55
1:B:1175:GLY:HA2	1:B:1221:VAL:O	2.07	0.55
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.04	0.54
1:B:1492:TRP:HZ3	1:B:1558:GLY:O	1.90	0.54
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.40	0.54
1:B:95:VAL:HG22	1:B:115:GLN:CG	2.37	0.54
1:B:323:ARG:CZ	1:B:468:PHE:HE2	2.16	0.54
1:A:582:ILE:HG23	1:A:653:ILE:HD11	1.89	0.54
1:A:1240:VAL:O	1:A:1243:ARG:HB2	2.07	0.54
1:B:1841:TYR:HE1	1:B:1846:MET:HE2	1.72	0.54
1:B:668:GLY:H	1:B:791:PRO:HA	1.73	0.54
1:B:1422:SER:HB3	1:B:1445:ASN:OD1	2.07	0.54
1:A:679:GLU:OE2	1:A:684:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1841:TYR:CE1	1:A:1846:MET:HE2	2.43	0.53
1:A:318:ASP:OD1	1:A:320:SER:OG	2.24	0.53
1:A:1657:TYR:CD2	1:A:1687:ARG:HG2	2.43	0.53
1:B:582:ILE:CG2	1:B:653:ILE:HD11	2.38	0.53
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.55	0.53
1:A:1365:MET:SD	1:A:1385:ILE:HD13	2.47	0.53
1:B:1469:PHE:O	1:B:1479:HIS:O	2.26	0.53
1:A:644:LEU:N	1:A:644:LEU:HD23	2.24	0.53
1:A:296:ALA:HB1	1:A:368:TYR:O	2.09	0.53
1:A:895:ASN:CG	1:A:898:LYS:HA	2.28	0.53
1:A:2085:ILE:HG13	1:B:1650:ASP:HA	1.90	0.53
1:B:1344:THR:HG21	1:B:1393:PHE:CZ	2.43	0.53
1:B:183:LEU:HD22	1:B:189:SER:OG	2.09	0.53
1:A:1648:ASN:O	1:A:1650:ASP:N	2.41	0.53
1:B:56:HIS:CD2	1:B:409:GLY:HA3	2.44	0.53
1:B:663:LEU:HG	1:B:676:TRP:HZ3	1.74	0.53
1:A:1657:TYR:CE2	1:A:1687:ARG:HG2	2.44	0.53
1:A:1753:PRO:HB3	1:A:1775:LEU:HD23	1.90	0.53
1:A:106:ASN:ND2	1:B:658:LEU:HB3	2.22	0.53
1:B:545:LYS:O	1:B:549:THR:HG23	2.08	0.53
1:A:1631:MET:CE	1:B:2034:LYS:HB3	2.39	0.53
1:A:585:ALA:HA	1:A:621:VAL:HG11	1.91	0.52
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.24	0.52
1:A:311:ASN:HB2	1:A:350:VAL:HG13	1.89	0.52
1:A:482:SER:HB2	1:B:487:TRP:HB2	1.91	0.52
1:B:1751:GLY:HA2	1:B:1775:LEU:HD21	1.91	0.52
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.39	0.52
1:B:1827:TRP:O	1:B:1829:ARG:N	2.42	0.52
1:A:550:GLU:HG3	1:A:554:ASP:OD2	2.10	0.52
1:B:584:GLY:HA2	1:B:685:LEU:HD11	1.90	0.52
1:A:864:GLU:OE1	1:A:868:ARG:NH1	2.43	0.52
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.57	0.52
1:A:67:ASN:ND2	1:A:128:TYR:CE2	2.77	0.52
1:A:1691:LYS:HA	1:A:1691:LYS:HE2	1.91	0.52
1:B:1762:ILE:O	1:B:1765:MET:HB2	2.10	0.52
1:B:1593:ILE:HG22	1:B:1593:ILE:O	2.10	0.52
1:A:297:ARG:HD2	1:A:320:SER:OG	2.10	0.52
1:A:56:HIS:CD2	1:A:409:GLY:HA3	2.44	0.52
1:B:1243:ARG:NH1	1:B:1283:TYR:O	2.42	0.52
1:A:69:ILE:O	1:A:70:ALA:C	2.47	0.52
1:B:990:GLN:HG3	1:B:991:PRO:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PHE:HD1	1:A:530:LEU:HD13	1.75	0.52
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	1.91	0.52
1:B:1759:ALA:H	1:B:1774:ASN:ND2	2.07	0.52
1:B:682:ALA:HB1	1:B:694:LEU:O	2.10	0.51
1:A:633:THR:HG23	1:A:645:PHE:HB2	1.91	0.51
1:B:1369:LEU:HD21	1:B:1415:LEU:HD23	1.91	0.51
1:A:2039:LYS:NZ	1:B:1633:GLU:OE1	2.33	0.51
1:A:66:ASN:HD22	1:A:67:ASN:H	1.56	0.51
1:A:1516:ARG:HG2	1:A:1537:PHE:CG	2.46	0.51
1:B:2183:ASP:HA	1:B:2186:LEU:HD12	1.92	0.51
1:A:581:VAL:HG12	1:A:632:PHE:CZ	2.45	0.51
1:A:220:VAL:CG2	1:A:355:LEU:HG	2.37	0.51
1:A:613:ASP:O	1:A:616:GLN:HB2	2.11	0.51
1:A:1727:LEU:HD12	1:A:1747:ILE:O	2.10	0.51
1:B:646:ILE:HG22	1:B:649:SER:OG	2.11	0.51
1:B:47:ARG:O	1:B:50:VAL:N	2.44	0.51
1:A:1493:LEU:HD11	1:A:1507:TYR:CE1	2.45	0.51
1:A:1841:TYR:CZ	1:A:1846:MET:HE3	2.45	0.51
1:B:387:GLU:CD	1:B:458:ARG:HH21	2.14	0.51
1:B:1333:ASP:OD2	1:B:1490:LYS:HB2	2.10	0.51
1:A:1842:ASP:O	1:A:1843:VAL:C	2.49	0.51
1:A:1315:THR:O	1:A:1317:ASN:N	2.43	0.51
1:A:975:VAL:O	1:A:976:SER:C	2.49	0.51
1:B:475:LEU:O	1:B:494:ASN:O	2.28	0.51
1:A:942:GLY:HA3	1:A:945:VAL:HG23	1.93	0.51
1:B:1827:TRP:CE3	1:B:1828:ASP:HA	2.46	0.51
1:A:2101:SER:HB2	1:B:1692:THR:HG21	1.93	0.50
1:A:1338:THR:HG21	1:A:1368:ILE:HG23	1.93	0.50
1:A:1353:ILE:HD12	1:A:1394:ASP:O	2.11	0.50
1:A:1404:PHE:O	1:A:1407:PHE:N	2.44	0.50
1:A:211:VAL:CG1	1:A:220:VAL:HG13	2.41	0.50
1:A:591:LEU:HD21	1:A:676:TRP:CZ2	2.47	0.50
1:A:668:GLY:HA2	1:A:790:SER:O	2.12	0.50
1:B:1223:ASN:HB3	1:B:1262:THR:HB	1.93	0.50
1:B:147:TRP:CH2	1:B:149:GLY:HA3	2.47	0.50
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.12	0.50
1:B:2026:GLU:O	1:B:2027:PRO:C	2.50	0.50
1:B:925:ILE:O	1:B:928:HIS:HB3	2.11	0.50
1:B:1763:ASN:OD1	1:B:1770:VAL:HG12	2.12	0.50
1:B:386:VAL:CG1	1:B:458:ARG:NH2	2.75	0.50
1:B:940:PHE:HA	1:B:950:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:PHE:HA	1:A:950:ILE:HD13	1.92	0.50
1:A:970:LEU:HA	1:A:973:SER:OG	2.12	0.50
1:B:561:TRP:CZ2	1:B:565:LEU:HD11	2.47	0.50
1:B:2033:ILE:O	1:B:2034:LYS:HD2	2.12	0.50
1:B:1616:ILE:HD12	1:B:1813:LYS:HB3	1.92	0.50
1:A:1643:TRP:CE3	1:A:1649:PRO:CB	2.94	0.50
1:B:1633:GLU:HA	1:B:1636:VAL:CG2	2.41	0.50
1:A:1708:SER:CB	1:B:2001:VAL:HG12	2.42	0.50
1:B:1451:VAL:HG22	1:B:1517:GLN:HG2	1.94	0.50
1:B:323:ARG:NH2	1:B:566:ILE:HG23	2.26	0.49
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.77	0.49
1:B:130:ASN:C	1:B:130:ASN:OD1	2.50	0.49
1:A:393:MET:CE	1:A:512:PHE:HB2	2.42	0.49
1:B:377:PHE:CZ	1:B:379:GLU:HA	2.47	0.49
1:A:1589:ILE:HG13	1:A:1589:ILE:O	2.12	0.49
1:B:1371:ASN:O	1:B:1375:THR:HG23	2.11	0.49
1:B:1493:LEU:HD11	1:B:1557:PRO:HB2	1.93	0.49
1:A:794:GLU:N	1:A:794:GLU:OE1	2.32	0.49
1:A:486:VAL:HG11	1:A:526:ALA:HB2	1.94	0.49
1:A:669:GLY:O	1:B:115:GLN:HB3	2.12	0.49
1:B:1603:PHE:O	1:B:1607:VAL:HG23	2.13	0.49
1:B:486:VAL:HG11	1:B:526:ALA:CB	2.43	0.49
1:A:108:GLU:HG2	1:A:111:ARG:NH2	2.28	0.49
1:B:1593:ILE:CG2	1:B:1731:ARG:NH2	2.76	0.49
1:B:1762:ILE:HG21	1:B:1771:TYR:HE1	1.77	0.49
1:B:2086:TYR:HA	1:B:2089:ILE:HD12	1.94	0.49
1:B:363:THR:HG21	1:B:385:GLN:OE1	2.13	0.49
1:A:1618:ARG:C	1:A:1619:ILE:HD12	2.33	0.49
1:B:1272:TYR:CD1	1:B:1318:ARG:HD2	2.47	0.49
1:B:1592:LYS:C	1:B:1594:GLY:H	2.15	0.49
1:A:601:ILE:O	1:A:602:GLU:C	2.51	0.49
1:B:323:ARG:NH2	1:B:566:ILE:HG12	2.27	0.49
1:A:2004:ASP:OD2	1:A:2006:THR:CG2	2.60	0.49
1:A:72:VAL:HA	1:A:112:MET:CE	2.43	0.49
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.78	0.49
1:A:393:MET:HE1	1:A:512:PHE:HB2	1.95	0.48
1:B:2083:LEU:O	1:B:2084:PRO:C	2.51	0.48
1:A:644:LEU:HD21	1:A:653:ILE:HD12	1.95	0.48
1:B:630:TYR:CE1	1:B:781:PHE:CD1	3.01	0.48
1:A:2047:LEU:HD13	1:B:1641:VAL:HG23	1.94	0.48
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1373:GLU:OE2	1:A:1414:ARG:NH2	2.42	0.48
1:A:1222:ALA:O	1:A:1261:ILE:HA	2.13	0.48
1:A:1779:GLY:HA3	1:A:1781:GLN:HE22	1.78	0.48
1:A:1103:GLN:O	1:A:1107:ARG:CG	2.61	0.48
1:B:927:VAL:HG13	1:B:1006:PRO:HG3	1.95	0.48
1:B:341:THR:HG21	1:B:368:TYR:HE1	1.78	0.48
1:B:1095:PRO:HA	1:B:1098:THR:HB	1.95	0.48
1:A:73:LYS:HE3	1:A:389:PRO:HG3	1.95	0.48
1:B:1408:LEU:HD22	1:B:1415:LEU:CD1	2.44	0.48
1:B:1925:HIS:H	1:B:1928:SER:HB3	1.77	0.48
1:B:865:LEU:HD12	1:B:868:ARG:NH2	2.28	0.48
1:B:150:TRP:CZ2	1:B:386:VAL:HG23	2.49	0.48
1:A:582:ILE:CG2	1:A:653:ILE:HD11	2.44	0.48
1:A:1772:THR:N	1:A:1776:GLN:OE1	2.44	0.48
1:B:1648:ASN:O	1:B:1651:LYS:HB2	2.13	0.48
1:A:485:ASN:OD1	1:A:522:HIS:NE2	2.47	0.48
1:B:1422:SER:CB	1:B:1445:ASN:OD1	2.61	0.48
1:A:1048:LEU:O	1:A:1051:SER:OG	2.26	0.48
1:B:1766:LEU:CD1	1:B:1770:VAL:HG11	2.41	0.47
1:A:654:ILE:HD12	1:A:792:VAL:CG2	2.43	0.47
1:B:1829:ARG:NH1	1:B:1858:TYR:HB3	2.29	0.47
1:B:684:ARG:HH11	1:B:684:ARG:CB	2.26	0.47
1:B:102:ASP:OD1	1:B:499:HIS:HE1	1.97	0.47
1:A:565:LEU:O	1:A:568:HIS:O	2.31	0.47
1:A:655:LEU:HD22	1:A:663:LEU:HD22	1.95	0.47
1:B:386:VAL:HG13	1:B:458:ARG:NH2	2.29	0.47
1:A:1576:TYR:CE1	1:A:1819:PRO:HB3	2.49	0.47
1:A:90:ARG:O	1:A:91:THR:C	2.52	0.47
1:A:1631:MET:HE3	1:B:2034:LYS:HB3	1.95	0.47
1:B:1544:GLU:OE1	1:B:1606:LYS:NZ	2.36	0.47
1:B:1180:VAL:CG1	1:B:1185:ASP:HB2	2.44	0.47
1:B:1497:ARG:O	1:B:1498:TYR:C	2.50	0.47
1:A:1709:GLY:O	1:A:1710:LEU:C	2.52	0.47
1:B:1030:ILE:HD13	1:B:1371:ASN:OD1	2.14	0.47
1:B:1408:LEU:HD12	1:B:1444:ILE:HG22	1.97	0.47
1:A:1633:GLU:HA	1:A:1636:VAL:HG23	1.97	0.47
1:A:1350:ASP:N	1:A:1350:ASP:OD1	2.48	0.47
1:A:178:ASN:OD1	1:A:179:ALA:N	2.48	0.47
1:A:687:VAL:HG12	1:A:688:ASP:OD2	2.15	0.47
1:B:1278:PHE:CE1	1:B:1285:GLU:HB2	2.50	0.47
1:B:322:GLN:O	1:B:562:LEU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:HD23	1:A:540:VAL:HG11	1.97	0.47
1:A:558:THR:H	1:A:561:TRP:HB2	1.78	0.47
1:B:1632:ALA:HB1	1:B:1634:GLU:OE1	2.15	0.47
1:A:1256:ALA:O	1:A:1257:SER:C	2.52	0.47
1:A:1180:VAL:HG13	1:A:1185:ASP:HB2	1.97	0.47
1:A:220:VAL:HG12	1:A:221:SER:N	2.30	0.47
1:A:250:MET:SD	1:A:264:GLN:HG2	2.54	0.47
1:A:480:PHE:HZ	1:A:486:VAL:HG12	1.80	0.46
1:B:46:LEU:O	1:B:50:VAL:HG23	2.15	0.46
1:A:1736:GLY:O	1:A:1740:VAL:HG23	2.15	0.46
1:A:150:TRP:CZ2	1:A:386:VAL:HG23	2.50	0.46
1:B:1365:MET:SD	1:B:1385:ILE:HD13	2.55	0.46
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.15	0.46
1:B:1258:ILE:O	1:B:1258:ILE:HG22	2.15	0.46
1:B:1408:LEU:HD22	1:B:1415:LEU:HD11	1.96	0.46
1:B:211:VAL:HG11	1:B:220:VAL:CG1	2.45	0.46
1:B:1770:VAL:CG1	1:B:1771:TYR:N	2.79	0.46
1:A:1981:TYR:CD2	1:A:1985:ILE:HD11	2.50	0.46
1:B:163:LEU:O	1:B:166:SER:HB3	2.14	0.46
1:B:1197:ILE:HD13	1:B:1256:ALA:HA	1.97	0.46
1:A:389:PRO:HB2	1:A:510:PHE:CE1	2.51	0.46
1:B:2022:ALA:HB3	1:B:2103:MET:CE	2.46	0.46
1:A:2044:MET:HE3	1:A:2082:LEU:HB2	1.97	0.46
1:A:1587:ASN:ND2	1:A:1620:TYR:OH	2.48	0.46
1:B:1180:VAL:HG13	1:B:1185:ASP:HB2	1.98	0.46
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.16	0.46
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.96	0.46
1:B:644:LEU:O	1:B:650:LYS:HA	2.15	0.46
1:A:646:ILE:HG21	1:A:785:LEU:HG	1.97	0.46
1:A:1783:MET:HE3	1:A:1788:VAL:HG11	1.98	0.46
1:A:891:ASN:HB3	1:A:894:TYR:HB2	1.97	0.46
1:A:76:ARG:HD3	1:B:529:GLU:OE2	2.15	0.46
1:A:1479:HIS:ND1	1:A:1480:LEU:HG	2.30	0.46
1:A:1571:VAL:O	1:A:1579:GLY:HA2	2.15	0.46
1:B:1909:ASN:HD22	1:B:1909:ASN:C	2.18	0.46
1:A:1652:GLY:HA2	1:B:2085:ILE:HD11	1.98	0.46
1:A:368:TYR:OH	1:A:370:HIS:CD2	2.68	0.46
1:A:1427:ILE:HG22	1:A:1428:ILE:N	2.30	0.46
1:B:1317:ASN:CB	1:B:1371:ASN:HD21	2.25	0.46
1:B:1592:LYS:O	1:B:1594:GLY:N	2.49	0.46
1:A:850:LEU:O	1:A:854:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ILE:HG22	1:A:667:ILE:O	2.15	0.46
1:B:498:ILE:HD12	1:B:536:PHE:CE2	2.51	0.46
1:B:301:VAL:CG1	1:B:313:SER:HB2	2.46	0.46
1:A:183:LEU:HD21	1:A:356:VAL:HG11	1.99	0.45
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.97	0.45
1:B:1493:LEU:HD21	1:B:1558:GLY:HA3	1.97	0.45
1:B:1492:TRP:CZ3	1:B:1558:GLY:O	2.69	0.45
1:B:646:ILE:HG23	1:B:647:ASN:N	2.31	0.45
1:B:1589:ILE:O	1:B:1589:ILE:HG13	2.17	0.45
1:A:1443:LEU:HD12	1:A:1443:LEU:N	2.31	0.45
1:B:646:ILE:CG2	1:B:649:SER:OG	2.64	0.45
1:B:458:ARG:O	1:B:543:LEU:HD11	2.16	0.45
1:A:905:GLU:HB3	1:A:906:PRO:HD3	1.97	0.45
1:A:993:CYS:SG	1:A:999:VAL:HG12	2.56	0.45
1:B:306:ASP:OD1	1:B:310:THR:HB	2.17	0.45
1:B:1657:TYR:HA	1:B:1690:ILE:HG12	1.99	0.45
1:B:55:GLY:HA2	1:B:409:GLY:O	2.16	0.45
1:A:299:LEU:HD13	1:A:334:VAL:HG11	1.97	0.45
1:A:1692:THR:HG21	1:B:2101:SER:HB2	1.99	0.45
1:A:485:ASN:HB2	1:A:522:HIS:HD2	1.80	0.45
1:B:1593:ILE:HG22	1:B:1731:ARG:HH21	1.81	0.45
1:A:988:HIS:HD2	1:A:989:TYR:CD2	2.34	0.45
1:B:1374:VAL:O	1:B:1374:VAL:HG12	2.16	0.45
1:B:822:MET:SD	1:B:981:LEU:CA	3.04	0.45
1:A:1827:TRP:CE3	1:A:1828:ASP:HA	2.52	0.45
1:B:35:LEU:HD23	1:B:169:LYS:HD2	1.99	0.45
1:A:72:VAL:HA	1:A:112:MET:HE1	1.98	0.45
1:A:132:ASP:CB	1:B:848:SER:OG	2.64	0.45
1:B:1592:LYS:C	1:B:1594:GLY:N	2.70	0.45
1:B:1808:SER:OG	1:B:1883:ARG:NH2	2.50	0.45
1:A:419:ARG:CZ	1:A:428:SER:O	2.65	0.45
1:B:150:TRP:NE1	1:B:386:VAL:HB	2.32	0.45
1:A:482:SER:HB3	1:B:482:SER:HB3	1.98	0.45
1:A:2154:ARG:O	1:A:2157:SER:OG	2.32	0.45
1:B:2131:ASN:HB3	1:B:2175:ILE:HG21	1.99	0.45
1:B:1352:SER:O	1:B:1353:ILE:C	2.54	0.45
1:A:1344:THR:HG21	1:A:1393:PHE:HZ	1.82	0.45
1:B:480:PHE:HD1	1:B:530:LEU:HD13	1.83	0.44
1:A:1045:GLU:HG3	1:A:1089:PHE:CE1	2.52	0.44
1:B:1135:LEU:HD23	1:B:1135:LEU:HA	1.85	0.44
1:B:1841:TYR:CE1	1:B:1846:MET:HE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:O	1:A:226:ILE:HG21	2.17	0.44
1:A:1757:THR:HG22	1:A:1762:ILE:HG13	1.98	0.44
1:A:1175:GLY:HA2	1:A:1221:VAL:O	2.17	0.44
1:B:1081:VAL:CG1	1:B:1084:ASP:OD1	2.66	0.44
1:B:1770:VAL:CG1	1:B:1771:TYR:CD1	3.00	0.44
1:A:1384:HIS:CD2	1:A:1385:ILE:N	2.86	0.44
1:A:1786:ASN:OD1	1:B:1964:PHE:O	2.35	0.44
1:B:1272:TYR:CE1	1:B:1318:ARG:HD2	2.52	0.44
1:A:1344:THR:HG21	1:A:1393:PHE:CZ	2.52	0.44
1:A:809:LEU:HD12	1:A:929:PHE:CE2	2.53	0.44
1:A:793:ILE:HD13	1:B:117:ILE:HD11	2.00	0.44
1:B:79:ARG:HG2	1:B:89:ASP:O	2.17	0.44
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.17	0.44
1:A:904:VAL:O	1:A:905:GLU:C	2.56	0.44
1:A:1619:ILE:HD12	1:A:1619:ILE:N	2.32	0.44
1:A:1027:GLU:O	1:A:1031:GLN:HG3	2.17	0.44
1:B:668:GLY:HA2	1:B:790:SER:O	2.17	0.44
1:B:319:CYS:HG	1:B:330:GLU:CD	2.17	0.44
1:A:1781:GLN:H	1:A:1781:GLN:CD	2.21	0.44
1:A:1701:GLY:HA2	1:B:2024:VAL:HG23	2.00	0.44
1:B:876:PHE:O	1:B:878:ALA:N	2.50	0.44
1:B:480:PHE:HZ	1:B:486:VAL:HG12	1.82	0.44
1:B:2141:HIS:O	1:B:2190:LYS:NZ	2.50	0.44
1:B:1460:VAL:HG12	1:B:1461:LYS:N	2.31	0.44
1:B:850:LEU:O	1:B:851:HIS:C	2.55	0.44
1:B:304:LEU:HD11	1:B:406:ILE:CD1	2.48	0.43
1:B:388:HIS:N	1:B:389:PRO:CD	2.81	0.43
1:A:1756:LEU:HD23	1:B:1963:MET:SD	2.58	0.43
1:A:2164:ASP:O	1:A:2165:HIS:C	2.57	0.43
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB2	2.53	0.43
1:B:1580:ARG:HG3	1:B:1580:ARG:HH11	1.83	0.43
1:A:1432:PRO:HG2	1:A:1433:GLN:H	1.83	0.43
1:B:2116:THR:HG22	1:B:2117:GLU:OE2	2.18	0.43
1:A:2128:ARG:HG3	1:A:2168:ASP:HA	2.01	0.43
1:A:1708:SER:HB2	1:B:2001:VAL:HG12	2.00	0.43
1:A:1444:ILE:HG23	1:A:1454:THR:HG22	1.99	0.43
1:B:1843:VAL:CG2	1:B:1878:VAL:HG21	2.48	0.43
1:B:1479:HIS:ND1	1:B:1480:LEU:HG	2.34	0.43
1:B:1341:ILE:HG23	1:B:1390:ILE:HD12	2.00	0.43
1:A:1995:LEU:HD12	1:A:1995:LEU:HA	1.85	0.43
1:A:1075:LEU:HD12	1:A:1075:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1703:GLU:OE1	1:B:1703:GLU:N	2.37	0.43
1:B:681:ALA:O	1:B:696:VAL:HG23	2.17	0.43
1:A:1766:LEU:HD12	1:A:1770:VAL:HG21	2.01	0.43
1:B:618:MET:HB3	1:B:618:MET:HE2	1.85	0.43
1:B:1374:VAL:O	1:B:1374:VAL:CG1	2.66	0.43
1:B:913:LYS:HD2	1:B:914:TYR:CE2	2.52	0.43
1:B:462:GLU:O	1:B:464:PRO:HD3	2.19	0.43
1:A:665:ILE:HD12	1:A:674:ILE:CD1	2.49	0.43
1:B:1841:TYR:HE1	1:B:1846:MET:CE	2.32	0.43
1:B:389:PRO:HA	1:B:392:GLU:HB2	2.01	0.43
1:B:1638:LEU:O	1:B:1658:LEU:HD22	2.18	0.43
1:A:942:GLY:HA3	1:A:945:VAL:CG2	2.48	0.43
1:B:386:VAL:HG13	1:B:458:ARG:HH21	1.84	0.43
1:A:1636:VAL:HB	1:A:1637:PRO:HD3	2.01	0.43
1:A:681:ALA:O	1:A:696:VAL:HG23	2.19	0.43
1:B:306:ASP:HA	1:B:406:ILE:HG23	2.01	0.43
1:B:941:ASN:ND2	1:B:1013:LEU:HA	2.14	0.43
1:B:186:LYS:O	1:B:190:THR:OG1	2.34	0.43
1:B:828:GLN:O	1:B:832:VAL:HG23	2.19	0.43
1:A:195:SER:HA	1:A:209:ASP:HB2	2.01	0.43
1:B:640:ASP:N	1:B:640:ASP:OD1	2.52	0.43
1:B:131:VAL:HG13	1:B:159:LEU:HA	2.00	0.43
1:B:1655:TYR:CD1	1:B:1689:VAL:HG13	2.54	0.42
1:A:878:ALA:HB3	1:A:915:SER:HA	2.01	0.42
1:B:634:VAL:HG13	1:B:644:LEU:CD2	2.49	0.42
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.33	0.42
1:A:1741:ARG:O	1:A:1744:GLN:N	2.51	0.42
1:A:575:PRO:O	1:A:576:ASP:C	2.58	0.42
1:B:2036:ARG:O	1:B:2037:ARG:C	2.57	0.42
1:B:1852:THR:HB	1:B:1855:GLY:O	2.19	0.42
1:B:124:ASN:N	1:B:124:ASN:HD22	2.18	0.42
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.19	0.42
1:A:1808:SER:O	1:A:1883:ARG:NH2	2.52	0.42
1:A:813:LEU:HA	1:A:978:LYS:HG2	2.01	0.42
1:B:624:ILE:HG12	1:B:629:ARG:HB2	2.00	0.42
1:B:1299:GLN:O	1:B:1388:ASN:ND2	2.47	0.42
1:B:1581:GLN:HB2	1:B:1616:ILE:HD11	2.00	0.42
1:B:1836:THR:HB	1:B:1839:GLU:HB2	2.00	0.42
1:B:1285:GLU:HG2	1:B:1287:GLU:HG2	2.01	0.42
1:B:1782:ILE:O	1:B:1786:ASN:HB2	2.19	0.42
1:B:1406:GLY:HA2	1:B:1409:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:PHE:CE2	1:B:783:GLY:O	2.73	0.42
1:A:1408:LEU:CD1	1:A:1444:ILE:HG22	2.49	0.42
1:A:384:LEU:HD11	1:A:388:HIS:CG	2.54	0.42
1:B:1365:MET:O	1:B:1369:LEU:HG	2.19	0.42
1:A:2159:TYR:CE1	1:A:2171:VAL:HG13	2.55	0.42
1:B:1670:ASP:OD1	1:B:1670:ASP:O	2.37	0.42
1:A:173:ILE:HG22	1:A:173:ILE:O	2.19	0.42
1:A:1593:ILE:O	1:A:1593:ILE:HG22	2.20	0.42
1:A:1404:PHE:O	1:A:1405:GLY:C	2.57	0.42
1:A:1408:LEU:HD12	1:A:1444:ILE:HG22	2.02	0.42
1:A:990:GLN:HG3	1:A:991:PRO:CD	2.50	0.42
1:A:1874:ALA:HB2	1:A:1927:ASN:HB2	2.02	0.42
1:A:835:ASN:OD1	1:A:837:LYS:HB2	2.20	0.42
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	2.01	0.42
1:B:368:TYR:CE2	1:B:370:HIS:HA	2.55	0.42
1:B:1539:SER:HB2	1:B:1569:ILE:HG12	2.02	0.42
1:B:95:VAL:HG22	1:B:115:GLN:HG3	2.02	0.42
1:B:297:ARG:HD3	1:B:320:SER:OG	2.19	0.42
1:B:323:ARG:CZ	1:B:566:ILE:CG1	2.94	0.41
1:A:1766:LEU:CD1	1:A:1770:VAL:HG21	2.50	0.41
1:A:658:LEU:HD22	1:B:106:ASN:OD1	2.20	0.41
1:A:35:LEU:O	1:A:35:LEU:HG	2.20	0.41
1:B:1682:ILE:HG22	1:B:1683:ASN:N	2.35	0.41
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.35	0.41
1:A:297:ARG:NH1	1:A:318:ASP:OD2	2.53	0.41
1:A:334:VAL:HG21	1:A:342:PHE:CE1	2.55	0.41
1:A:990:GLN:HG3	1:A:991:PRO:N	2.35	0.41
1:A:73:LYS:HB2	1:A:489:TYR:CE1	2.55	0.41
1:B:1724:THR:O	1:B:1745:ARG:HB2	2.20	0.41
1:A:1703:GLU:OE2	1:A:1703:GLU:N	2.36	0.41
1:A:2086:TYR:HA	1:A:2089:ILE:HD13	2.01	0.41
1:A:2041:LEU:HD13	1:A:2051:TYR:OH	2.19	0.41
1:A:311:ASN:N	1:A:311:ASN:HD22	2.18	0.41
1:B:297:ARG:CD	1:B:320:SER:OG	2.67	0.41
1:B:1011:VAL:HG11	1:B:1026:ARG:NH2	2.35	0.41
1:A:2093:PHE:O	1:A:2097:HIS:HD2	2.03	0.41
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.84	0.41
1:B:1044:ILE:HD13	1:B:1075:LEU:HD22	2.01	0.41
1:B:69:ILE:HG23	1:B:489:TYR:CE1	2.55	0.41
1:A:799:ALA:HB1	1:A:845:LEU:HD12	2.02	0.41
1:B:210:THR:O	1:B:226:ILE:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1738:TYR:O	1:B:1742:LEU:HD22	2.20	0.41
1:A:1640:GLN:HB3	1:A:1657:TYR:CZ	2.55	0.41
1:A:1842:ASP:O	1:A:1844:ARG:N	2.54	0.41
1:B:1732:SER:OG	1:B:1736:GLY:C	2.59	0.41
1:B:2128:ARG:HG3	1:B:2168:ASP:HA	2.02	0.41
1:B:1639:PHE:C	1:B:1639:PHE:CD1	2.93	0.41
1:B:323:ARG:NH2	1:B:566:ILE:CG2	2.83	0.41
1:A:1569:ILE:HG22	1:A:1571:VAL:CG2	2.51	0.41
1:B:1825:ASP:OD2	1:B:1825:ASP:C	2.59	0.41
1:B:147:TRP:CZ2	1:B:149:GLY:HA2	2.55	0.41
1:A:90:ARG:C	1:A:92:VAL:N	2.72	0.41
1:A:1603:PHE:O	1:A:1607:VAL:HG23	2.21	0.41
1:A:1835:PRO:CG	1:A:1846:MET:CE	2.93	0.41
1:A:1624:ASN:ND2	1:A:1732:SER:HA	2.36	0.41
1:B:1471:SER:HB2	1:B:1479:HIS:HD2	1.86	0.41
1:A:1629:ILE:HG22	1:B:2024:VAL:HG11	2.03	0.41
1:A:696:VAL:O	1:A:696:VAL:HG12	2.20	0.41
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.51	0.41
1:B:802:PHE:O	1:B:806:VAL:HG23	2.20	0.41
1:B:1225:CYS:HB2	1:B:1264:MET:HE3	2.03	0.41
1:A:1852:THR:HG22	1:A:1853:GLU:N	2.35	0.41
1:B:933:TYR:OH	1:B:979:ASN:ND2	2.53	0.41
1:A:412:MET:HG3	1:A:418:ILE:HG21	2.03	0.41
1:A:220:VAL:CG1	1:A:221:SER:N	2.84	0.41
1:A:2037:ARG:O	1:A:2041:LEU:HB2	2.21	0.41
1:B:1322:VAL:HG22	1:B:1338:THR:HG23	2.02	0.41
1:B:2115:TRP:O	1:B:2116:THR:C	2.58	0.41
1:A:334:VAL:HG21	1:A:342:PHE:HE1	1.86	0.41
1:A:2159:TYR:OH	1:A:2175:ILE:HD11	2.21	0.41
1:B:1232:PHE:CE1	1:B:1241:ARG:HG3	2.55	0.41
1:B:2079:GLU:C	1:B:2081:GLU:H	2.25	0.41
1:B:1052:VAL:HG12	1:B:1053:VAL:N	2.36	0.41
1:B:196:ALA:HB2	1:B:355:LEU:HD22	2.03	0.41
1:A:389:PRO:HA	1:A:392:GLU:HB2	2.03	0.40
1:B:2138:ARG:NH2	1:B:2183:ASP:OD2	2.54	0.40
1:B:684:ARG:HH11	1:B:684:ARG:HB3	1.85	0.40
1:A:2013:GLU:OE1	1:A:2129:ARG:HD3	2.21	0.40
1:B:202:PRO:HB2	1:B:291:LYS:HB2	2.03	0.40
1:B:835:ASN:HD22	1:B:836:PRO:HD2	1.86	0.40
1:B:1783:MET:CA	1:B:1786:ASN:HB2	2.45	0.40
1:B:1657:TYR:HB3	1:B:1689:VAL:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1960:GLN:HE21	1:B:1960:GLN:HB2	1.64	0.40
1:B:1100:ALA:O	1:B:1103:GLN:HB2	2.20	0.40
1:B:1783:MET:HE1	1:B:1788:VAL:HG21	2.02	0.40
1:A:1182:HIS:CE1	1:A:1230:GLU:O	2.71	0.40
1:B:1239:LEU:O	1:B:1243:ARG:HG2	2.21	0.40
1:B:1649:PRO:C	1:B:1651:LYS:H	2.24	0.40
1:A:625:HIS:O	1:A:626:GLU:HB2	2.21	0.40
1:A:1940:ASN:ND2	1:A:1981:TYR:HA	2.37	0.40
1:A:1620:TYR:O	1:A:1726:THR:HA	2.21	0.40
1:B:1544:GLU:HA	1:B:1549:GLU:O	2.22	0.40
1:A:955:ARG:NH2	1:A:1914:GLU:OE1	2.46	0.40
1:A:596:ALA:HB1	1:A:614:LEU:O	2.21	0.40
1:B:323:ARG:CZ	1:B:468:PHE:CZ	3.04	0.40
1:A:486:VAL:HG11	1:A:526:ALA:HB1	2.01	0.40
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.03	0.40
1:A:185:ASP:OD2	1:A:227:TYR:OH	2.27	0.40
1:A:2058:LEU:HD21	1:A:2071:ILE:HB	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:440:ASP:OD1	1:A:440:ASP:OD1[7_466]	1.80	0.40

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	1980/2218 (89%)	1771 (89%)	188 (10%)	21 (1%)	17	55
1	B	1997/2218 (90%)	1778 (89%)	203 (10%)	16 (1%)	24	63
All	All	3977/4436 (90%)	3549 (89%)	391 (10%)	37 (1%)	21	61

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	572	ALA
1	A	184	GLY
1	A	573	GLU
1	A	1316	ASP
1	A	1378	SER
1	A	1591	PHE
1	A	1843	VAL
1	B	184	GLY
1	B	1593	ILE
1	B	1682	ILE
1	A	431	GLU
1	A	1050	SER
1	A	1828	ASP
1	B	1650	ASP
1	B	1744	GLN
1	B	2177	GLU
1	A	1098	THR
1	B	431	GLU
1	B	659	SER
1	B	689	SER
1	B	787	ASP
1	B	851	HIS
1	A	169	LYS
1	A	610	LEU
1	A	689	SER
1	A	898	LYS
1	A	1195	GLU
1	A	1305	LEU
1	A	1731	ARG
1	A	2166	GLU
1	B	1052	VAL
1	B	1769	GLU
1	B	1843	VAL
1	B	2080	ARG
1	A	680	VAL
1	A	783	GLY
1	A	1281	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	1718/1912 (90%)	1616 (94%)	102 (6%)	24	60
1	B	1735/1912 (91%)	1619 (93%)	116 (7%)	20	56
All	All	3453/3824 (90%)	3235 (94%)	218 (6%)	22	58

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	66	ASN
1	A	118	GLU
1	A	124	ASN
1	A	185	ASP
1	A	195	SER
1	A	221	SER
1	A	269	GLU
1	A	326	GLN
1	A	354	LYS
1	A	360	SER
1	A	391	THR
1	A	471	SER
1	A	477	GLU
1	A	479	ASN
1	A	489	TYR
1	A	508	HIS
1	A	537	ARG
1	A	602	GLU
1	A	629	ARG
1	A	633	THR
1	A	643	THR
1	A	644	LEU
1	A	659	SER
1	A	671	SER
1	A	779	LEU
1	A	790	SER

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Mol	Chain	Res	Type
1	A	793	ILE
1	A	796	THR
1	A	797	LYS
1	A	807	SER
1	A	841	SER
1	A	845	LEU
1	A	852	SER
1	A	883	LYS
1	A	915	SER
1	A	979	ASN
1	A	980	ASN
1	A	990	GLN
1	A	1044	ILE
1	A	1190	LEU
1	A	1191	SER
1	A	1193	SER
1	A	1223	ASN
1	A	1259	ARG
1	A	1282	ASN
1	A	1343	ARG
1	A	1350	ASP
1	A	1364	LEU
1	A	1390	ILE
1	A	1413	LYS
1	A	1417	ARG
1	A	1419	ARG
1	A	1433	GLN
1	A	1434	THR
1	A	1474	LYS
1	A	1536	PHE
1	A	1546	GLU
1	A	1583	VAL
1	A	1585	VAL
1	A	1592	LYS
1	A	1602	GLU
1	A	1624	ASN
1	A	1639	PHE
1	A	1660	SER
1	A	1686	GLU
1	A	1691	LYS
1	A	1726	THR
1	A	1732	SER

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Mol	Chain	Res	Type
1	A	1735	ILE
1	A	1755	ILE
1	A	1777	LEU
1	A	1781	GLN
1	A	1791	LEU
1	A	1792	THR
1	A	1797	LEU
1	A	1824	LYS
1	A	1843	VAL
1	A	1854	SER
1	A	1884	LEU
1	A	1912	SER
1	A	1924	TRP
1	A	1930	PHE
1	A	1968	LEU
1	A	1991	PRO
1	A	2001	VAL
1	A	2018	VAL
1	A	2021	ARG
1	A	2025	LEU
1	A	2027	PRO
1	A	2035	PHE
1	A	2041	LEU
1	A	2083	LEU
1	A	2090	SER
1	A	2117	GLU
1	A	2119	ARG
1	A	2127	ARG
1	A	2128	ARG
1	A	2149	LEU
1	A	2183	ASP
1	A	2186	LEU
1	A	2187	LYS
1	B	37	THR
1	B	66	ASN
1	B	108	GLU
1	B	124	ASN
1	B	195	SER
1	B	269	GLU
1	B	319	CYS
1	B	335	THR
1	B	360	SER

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Mol	Chain	Res	Type
1	B	367	LEU
1	B	417	ASP
1	B	457	CYS
1	B	471	SER
1	B	483	SER
1	B	508	HIS
1	B	531	SER
1	B	545	LYS
1	B	616	GLN
1	B	633	THR
1	B	643	THR
1	B	673	THR
1	B	684	ARG
1	B	782	GLU
1	B	784	MET
1	B	785	LEU
1	B	801	LYS
1	B	835	ASN
1	B	845	LEU
1	B	848	SER
1	B	853	ARG
1	B	882	SER
1	B	883	LYS
1	B	886	ASP
1	B	924	SER
1	B	967	LEU
1	B	975	VAL
1	B	990	GLN
1	B	997	SER
1	B	1015	SER
1	B	1040	ARG
1	B	1057	TYR
1	B	1084	ASP
1	B	1108	ARG
1	B	1180	VAL
1	B	1190	LEU
1	B	1191	SER
1	B	1223	ASN
1	B	1259	ARG
1	B	1343	ARG
1	B	1344	THR
1	B	1350	ASP

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Mol	Chain	Res	Type
1	B	1359	SER
1	B	1364	LEU
1	B	1380	SER
1	B	1390	ILE
1	B	1409	GLU
1	B	1419	ARG
1	B	1426	ARG
1	B	1430	LYS
1	B	1434	THR
1	B	1437	PRO
1	B	1474	LYS
1	B	1506	THR
1	B	1508	VAL
1	B	1521	SER
1	B	1533	THR
1	B	1534	ASP
1	B	1539	SER
1	B	1542	LEU
1	B	1546	GLU
1	B	1550	LEU
1	B	1568	LYS
1	B	1571	VAL
1	B	1580	ARG
1	B	1585	VAL
1	B	1634	GLU
1	B	1639	PHE
1	B	1648	ASN
1	B	1651	LYS
1	B	1653	PHE
1	B	1664	GLU
1	B	1665	THR
1	B	1667	LYS
1	B	1681	VAL
1	B	1683	ASN
1	B	1731	ARG
1	B	1735	ILE
1	B	1741	ARG
1	B	1742	LEU
1	B	1764	LYS
1	B	1769	GLU
1	B	1781	GLN
1	B	1786	ASN

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Mol	Chain	Res	Type
1	B	1802	LYS
1	B	1808	SER
1	B	1838	ASP
1	B	1843	VAL
1	B	1875	LYS
1	B	1889	LEU
1	B	1909	ASN
1	B	1915	THR
1	B	1920	PRO
1	B	1924	TRP
1	B	1930	PHE
1	B	1945	LEU
1	B	1960	GLN
1	B	1980	ASP
1	B	1992	THR
1	B	2030	MET
1	B	2035	PHE
1	B	2037	ARG
1	B	2101	SER
1	B	2106	LYS
1	B	2128	ARG
1	B	2162	SER
1	B	2192	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	124	ASN
1	A	152	HIS
1	A	280	ASN
1	A	343	HIS
1	A	370	HIS
1	A	445	GLN
1	A	453	HIS
1	A	979	ASN
1	A	988	HIS
1	A	1134	GLN
1	A	1182	HIS
1	A	1321	HIS
1	A	1384	HIS
1	A	1479	HIS

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Mol	Chain	Res	Type
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1648	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1781	GLN
1	A	1944	GLN
1	A	2060	ASN
1	A	2097	HIS
1	B	53	HIS
1	B	66	ASN
1	B	124	ASN
1	B	152	HIS
1	B	228	GLN
1	B	280	ASN
1	B	370	HIS
1	B	381	ASN
1	B	445	GLN
1	B	453	HIS
1	B	499	HIS
1	B	508	HIS
1	B	522	HIS
1	B	616	GLN
1	B	835	ASN
1	B	941	ASN
1	B	979	ASN
1	B	988	HIS
1	B	1092	HIS
1	B	1134	GLN
1	B	1479	HIS
1	B	1522	GLN
1	B	1560	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1774	ASN
1	B	1781	GLN
1	B	1786	ASN
1	B	1909	ASN
1	B	1941	ASN

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Mol	Chain	Res	Type
1	B	1960	GLN
1	B	2011	GLN
1	B	2057	GLN
1	B	2074	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

5.7   Other polymers (i)

There are no such residues in this entry.

5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1996/2218 (89%)	-0.15	38 (1%)	70	48	47, 85, 140, 237	0
1	B	2017/2218 (90%)	-0.05	78 (3%)	43	21	46, 87, 161, 237	0
All	All	4013/4436 (90%)	-0.10	116 (2%)	55	31	46, 86, 150, 237	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	897	ASP	6.7
1	A	856	ALA	6.4
1	B	293	ALA	6.4
1	A	897	ASP	5.8
1	B	2191	LEU	5.7
1	B	274	LEU	5.1
1	A	440	ASP	5.0
1	A	899	LEU	4.9
1	B	2182	LEU	4.9
1	B	289	ILE	4.6
1	B	264	GLN	4.5
1	B	278	ALA	4.5
1	A	441	ALA	4.5
1	B	242	ALA	4.4
1	A	439	GLN	4.3
1	B	245	ILE	4.3
1	B	899	LEU	4.3
1	B	292	LEU	4.2
1	B	267	ARG	4.1
1	A	442	THR	4.1
1	B	282	ILE	4.0
1	A	894	TYR	3.9
1	B	230	GLY	3.9
1	B	250	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	445	GLN	3.7
1	B	2181	THR	3.6
1	A	885	ILE	3.6
1	B	447	ARG	3.6
1	A	445	GLN	3.6
1	A	1465	GLY	3.6
1	A	2065	PRO	3.6
1	B	265	VAL	3.5
1	B	244	ARG	3.5
1	A	1464	LYS	3.5
1	B	240	GLN	3.4
1	B	2141	HIS	3.4
1	B	266	GLU	3.4
1	B	272	ILE	3.4
1	B	287	ILE	3.4
1	B	2188	GLY	3.3
1	A	438	THR	3.3
1	B	243	LYS	3.3
1	B	288	PHE	3.3
1	B	439	GLN	3.3
1	A	444	LYS	3.3
1	A	443	LYS	3.3
1	B	262	ILE	3.2
1	B	2161	ALA	3.1
1	B	443	LYS	3.1
1	A	902	ALA	3.1
1	B	226	ILE	3.1
1	B	444	LYS	3.1
1	A	889	VAL	3.1
1	B	2192	GLU	3.0
1	A	2181	THR	3.0
1	B	248	PRO	3.0
1	B	252	LYS	3.0
1	B	256	GLY	2.9
1	B	2158	TRP	2.9
1	A	2063	LEU	2.8
1	B	2190	LYS	2.8
1	B	231	CYS	2.8
1	B	254	SER	2.8
1	B	437	LYS	2.8
1	B	261	GLY	2.8
1	B	39	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	232	CYS	2.8
1	A	777	HIS	2.8
1	A	896	PRO	2.7
1	A	437	LYS	2.7
1	B	2193	SER	2.7
1	B	896	PRO	2.7
1	B	276	HIS	2.7
1	B	446	ARG	2.7
1	B	2189	LEU	2.7
1	A	2054	LEU	2.6
1	A	2184	ASP	2.6
1	A	2182	LEU	2.6
1	B	441	ALA	2.6
1	A	2057	GLN	2.6
1	A	2179	TYR	2.5
1	B	440	ASP	2.5
1	B	247	PHE	2.5
1	A	2185	LYS	2.5
1	B	295	ARG	2.5
1	B	779	LEU	2.5
1	B	294	GLY	2.5
1	B	894	TYR	2.5
1	A	2058	LEU	2.4
1	B	2185	LYS	2.4
1	B	271	PHE	2.4
1	B	225	ASP	2.3
1	B	241	LYS	2.3
1	A	888	ALA	2.3
1	B	436	PHE	2.3
1	B	260	LYS	2.3
1	A	236	GLU	2.3
1	B	434	PHE	2.3
1	B	41	LEU	2.3
1	A	854	LEU	2.3
1	B	36	ASN	2.3
1	B	268	GLU	2.2
1	B	438	THR	2.2
1	B	291	LYS	2.2
1	B	2068	HIS	2.2
1	A	855	PRO	2.1
1	A	2055	ARG	2.1
1	B	2140	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2066	GLU	2.1
1	B	432	ILE	2.1
1	B	569	LYS	2.1
1	B	270	ASP	2.1
1	B	281	GLU	2.1
1	A	2161	ALA	2.0
1	A	876	PHE	2.0
1	B	2187	LYS	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.