Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:13 PM GMT

PDB ID	:	1SMQ
Title	:	Structure of the Ribonucleotide Reductase Rnr2 Homodimer from Saccharomyces cerevisiae
Authors	:	Sommerhalter, M.; Voegtli, W.C.; Perlstein, D.L.; Ge, J.; Stubbe, J.; Rosenzweig, A.C.
Deposited on	:	2004-03-09
Resolution	:	3.10 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:

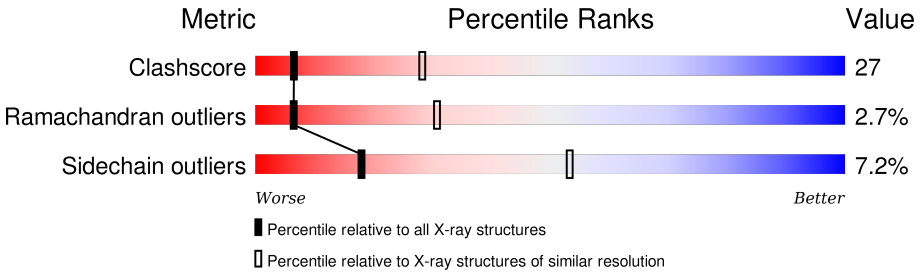
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.10 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	399	43% 36% • • 18%
1	B	399	43% 34% 5% • 18%
1	C	399	40% 35% • • 20%
1	D	399	40% 35% • • 20%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10690 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 Ribonucleoside-diphosphate reductase small chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2723	1757	449	506	11			
1	B	329	Total	C	N	O	S	0	0	0
			2723	1757	449	506	11			
1	C	318	Total	C	N	O	S	0	0	0
			2622	1693	426	492	11			
1	D	318	Total	C	N	O	S	0	0	0
			2622	1693	426	492	11			

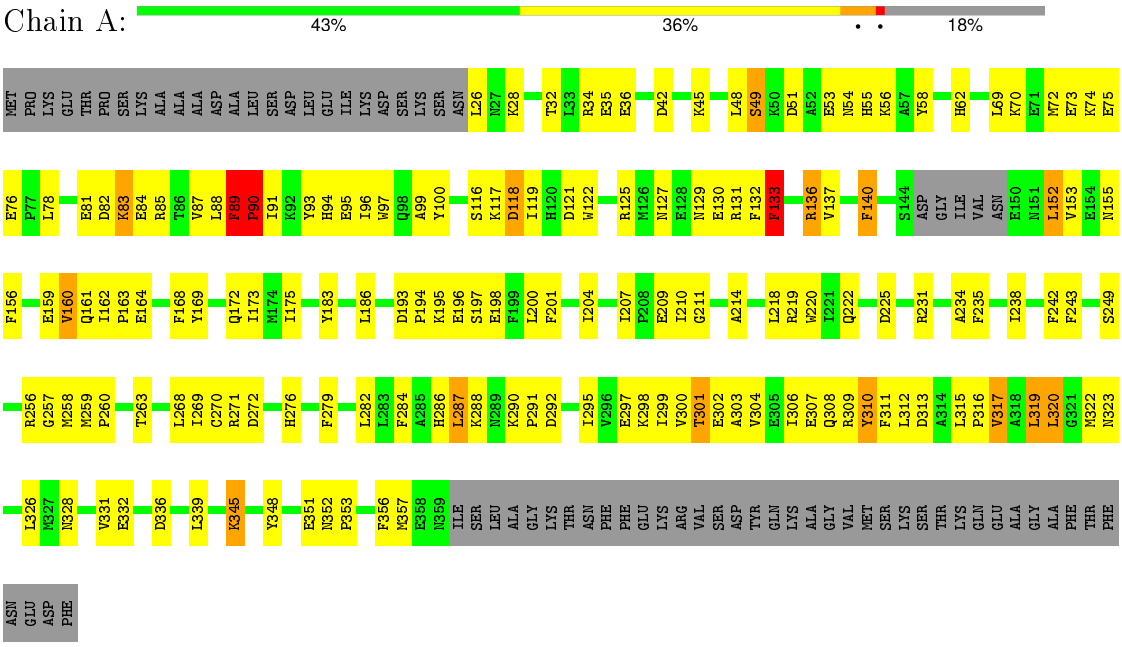
3 Residue-property plots (i)

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.

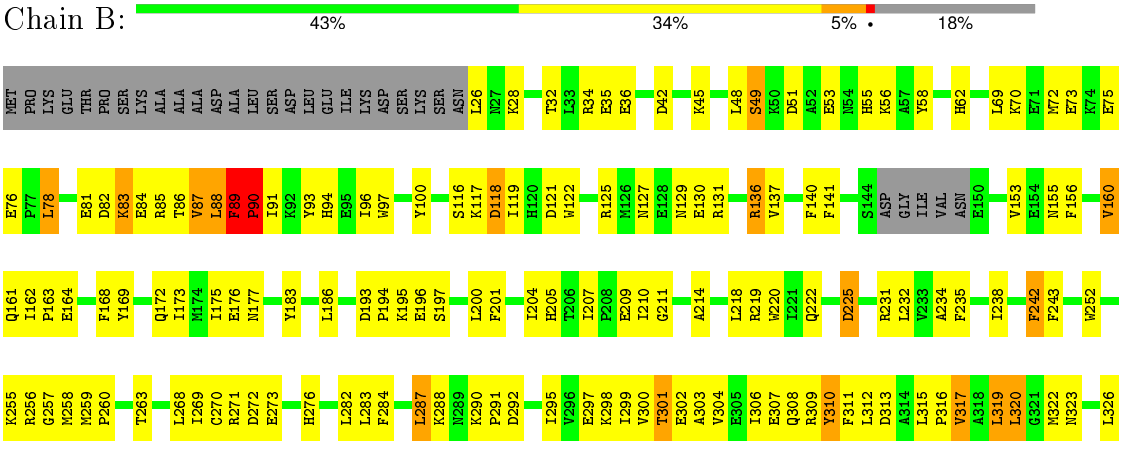
- Molecule 1: Ribonucleoside-diphosphate reductase small chain 1

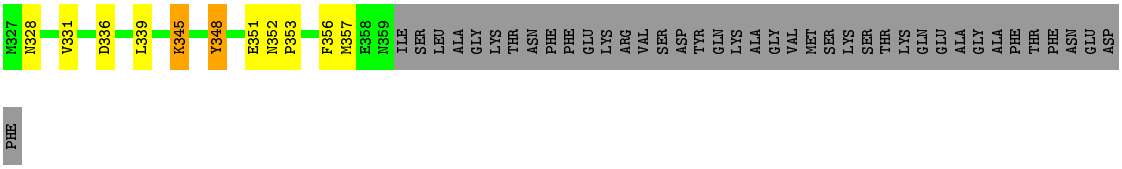
Chain A:



- Molecule 1: Ribonucleoside-diphosphate reductase small chain 1

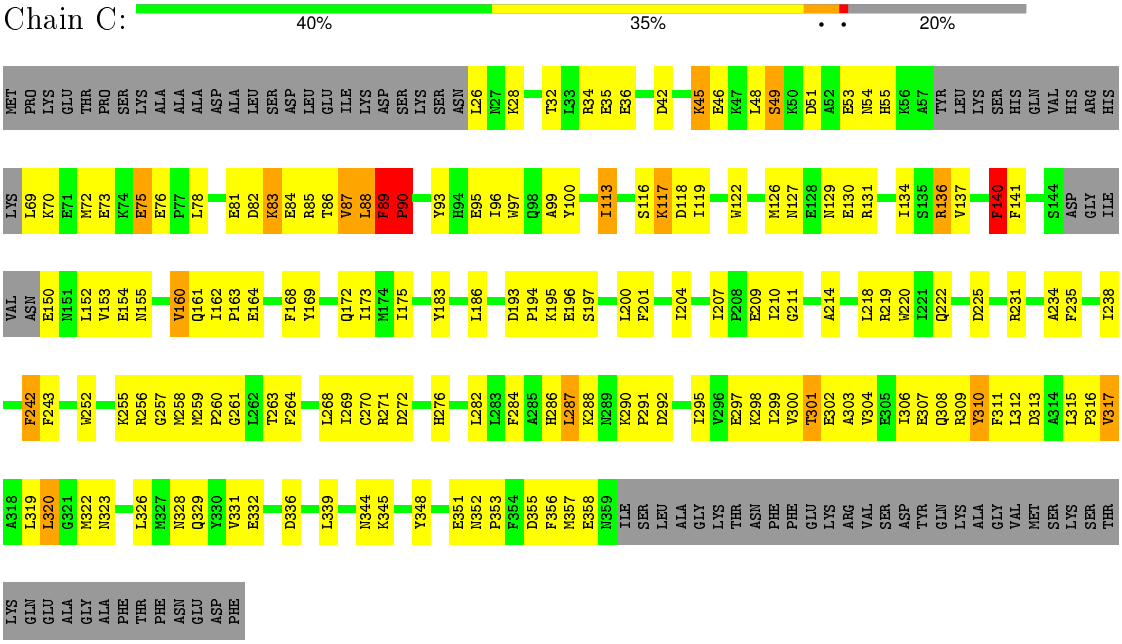
Chain B:





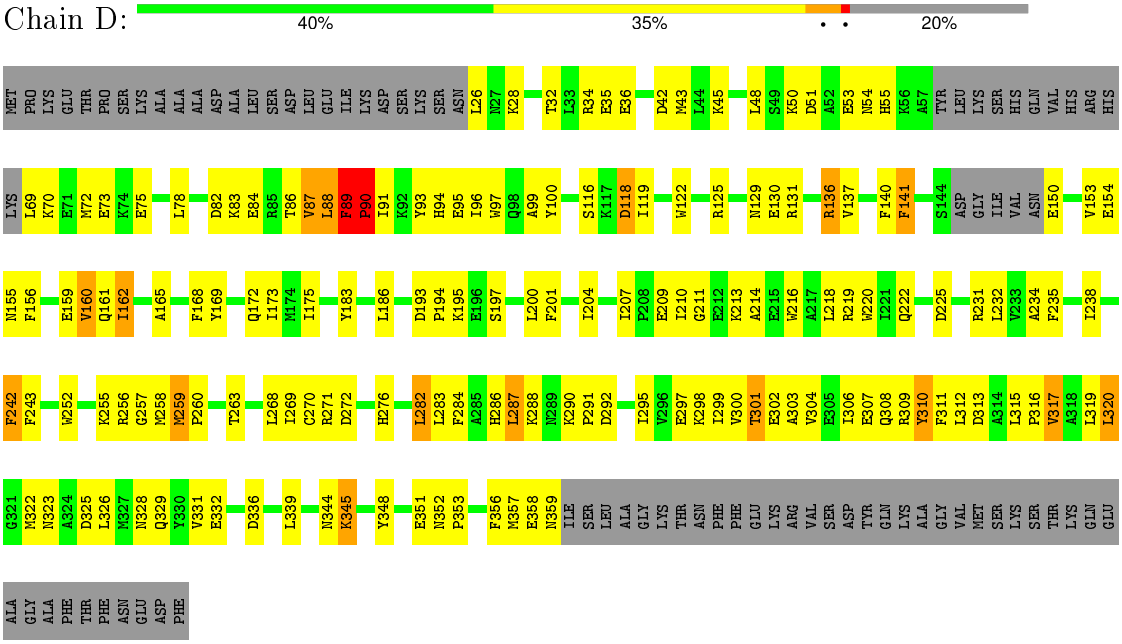
• Molecule 1: Ribonucleoside-diphosphate reductase small chain 1

Chain C:



• Molecule 1: Ribonucleoside-diphosphate reductase small chain 1

Chain D:



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	79.67Å 79.57Å 88.05Å 83.47° 83.45° 70.79°	Depositor
Resolution (Å)	25.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.272 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10690	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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	1/2788 (0.0%)	0.79	9/3759 (0.2%)
1	B	0.53	1/2788 (0.0%)	0.81	6/3759 (0.2%)
1	C	0.47	0/2682	0.79	6/3616 (0.2%)
1	D	0.49	0/2682	0.80	6/3616 (0.2%)
All	All	0.50	2/10940 (0.0%)	0.80	27/14750 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	3
1	D	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	PHE	CD2-CE2	-7.09	1.25	1.39
1	B	89	PHE	C-N	5.18	1.44	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	PHE	CB-CG-CD1	11.20	128.64	120.80
1	D	89	PHE	C-N-CD	9.51	148.38	128.40
1	A	89	PHE	C-N-CD	9.34	148.01	128.40
1	B	348	TYR	CB-CG-CD1	9.18	126.51	121.00
1	C	89	PHE	C-N-CD	9.09	147.48	128.40
1	B	89	PHE	C-N-CD	8.80	146.88	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	PHE	CD1-CG-CD2	-7.00	109.21	118.30
1	D	90	PRO	CA-N-CD	-6.77	102.03	111.50
1	A	133	PHE	CG-CD2-CE2	6.37	127.80	120.80
1	C	140	PHE	CB-CG-CD2	6.22	125.15	120.80
1	D	320	LEU	CA-CB-CG	6.11	129.35	115.30
1	C	320	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	140	PHE	CB-CG-CD1	6.07	125.05	120.80
1	B	320	LEU	CA-CB-CG	6.03	129.16	115.30
1	D	162	ILE	C-N-CD	5.99	140.97	128.40
1	A	320	LEU	CA-CB-CG	5.96	129.01	115.30
1	C	140	PHE	CB-CG-CD1	-5.88	116.69	120.80
1	D	141	PHE	CB-CG-CD1	5.74	124.82	120.80
1	C	90	PRO	CA-N-CD	-5.58	103.69	111.50
1	A	90	PRO	CA-N-CD	-5.57	103.70	111.50
1	A	133	PHE	CE1-CZ-CE2	-5.55	110.00	120.00
1	D	259	MET	C-N-CD	5.46	139.87	128.40
1	B	162	ILE	C-N-CD	5.44	139.82	128.40
1	A	140	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	B	90	PRO	CA-N-CD	-5.30	104.07	111.50
1	C	345	LYS	CB-CA-C	-5.07	100.27	110.40
1	B	345	LYS	CB-CA-C	-5.06	100.28	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	PHE	Sidechain
1	A	49	SER	Mainchain
1	B	348	TYR	Sidechain
1	B	49	SER	Mainchain
1	B	89	PHE	Mainchain
1	C	140	PHE	Mainchain
1	C	49	SER	Mainchain
1	C	89	PHE	Mainchain
1	D	161	GLN	Mainchain

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	2723	0	2660	156	3
1	B	2723	0	2660	138	0
1	C	2622	0	2557	151	3
1	D	2622	0	2557	141	0
All	All	10690	0	10434	579	3

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 27.

All (579) 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:D:153:VAL:HG22	1:D:173:ILE:HD13	1.15	1.13
1:B:153:VAL:HG22	1:B:173:ILE:HD13	1.32	1.11
1:A:153:VAL:HG22	1:A:173:ILE:HD13	1.24	1.10
1:C:153:VAL:HG22	1:C:173:ILE:HD13	1.13	1.10
1:A:292:ASP:HB3	1:A:295:ILE:HD13	1.37	1.05
1:D:292:ASP:HB3	1:D:295:ILE:HD13	1.40	1.04
1:B:78:LEU:HD21	1:B:283:LEU:HD22	1.40	1.04
1:C:292:ASP:HB3	1:C:295:ILE:HD13	1.40	1.04
1:B:292:ASP:HB3	1:B:295:ILE:HD13	1.40	1.02
1:D:155:ASN:HD21	1:D:231:ARG:HD2	1.30	0.95
1:C:153:VAL:HG22	1:C:173:ILE:CD1	1.97	0.94
1:A:89:PHE:O	1:A:90:PRO:C	2.01	0.94
1:D:153:VAL:HG22	1:D:173:ILE:CD1	1.97	0.94
1:D:87:VAL:HG21	1:D:90:PRO:HG2	1.52	0.92
1:C:323:ASN:HD22	1:C:326:LEU:HG	1.35	0.91
1:D:323:ASN:HD22	1:D:326:LEU:HG	1.35	0.91
1:B:323:ASN:HD22	1:B:326:LEU:HG	1.35	0.91
1:A:323:ASN:HD22	1:A:326:LEU:HG	1.36	0.91
1:B:48:LEU:O	1:B:51:ASP:HB2	1.72	0.89
1:B:93:TYR:HB3	1:B:96:ILE:HD13	1.55	0.88
1:D:95:GLU:OE2	1:D:95:GLU:HA	1.72	0.88
1:C:89:PHE:O	1:C:90:PRO:C	2.10	0.87
1:D:259:MET:O	1:D:263:THR:HG23	1.75	0.87
1:D:140:PHE:HE1	1:D:207:ILE:HD13	1.40	0.86
1:D:89:PHE:O	1:D:90:PRO:C	2.08	0.86
1:B:172:GLN:HE22	1:B:235:PHE:HZ	1.23	0.86
1:A:172:GLN:HE22	1:A:235:PHE:HZ	1.22	0.85
1:C:86:THR:O	1:C:88:LEU:HB2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:O	1:B:90:PRO:C	2.12	0.85
1:A:317:VAL:HB	1:A:322:MET:HB2	1.59	0.85
1:C:172:GLN:HE22	1:C:235:PHE:HZ	1.24	0.84
1:D:95:GLU:HG3	1:D:282:LEU:HD21	1.57	0.84
1:B:317:VAL:HB	1:B:322:MET:HB2	1.59	0.83
1:D:317:VAL:HB	1:D:322:MET:HB2	1.60	0.83
1:D:89:PHE:O	1:D:90:PRO:O	1.94	0.83
1:D:172:GLN:HE22	1:D:235:PHE:HZ	1.24	0.81
1:C:298:LYS:HE3	1:C:302:GLU:OE1	1.80	0.81
1:C:317:VAL:HB	1:C:322:MET:HB2	1.60	0.81
1:D:155:ASN:ND2	1:D:231:ARG:HD2	1.95	0.81
1:D:298:LYS:HE3	1:D:302:GLU:OE1	1.80	0.81
1:A:298:LYS:HE3	1:A:302:GLU:OE1	1.80	0.81
1:C:93:TYR:HB3	1:C:96:ILE:HD13	1.61	0.81
1:B:298:LYS:HE3	1:B:302:GLU:OE1	1.79	0.80
1:A:93:TYR:HB3	1:A:96:ILE:HD13	1.64	0.79
1:D:87:VAL:CG2	1:D:90:PRO:HG2	2.12	0.78
1:B:89:PHE:O	1:B:90:PRO:O	2.02	0.78
1:C:153:VAL:CG2	1:C:173:ILE:HD13	2.05	0.77
1:C:259:MET:O	1:C:263:THR:HG23	1.84	0.77
1:A:45:LYS:HB2	1:A:309:ARG:HE	1.49	0.77
1:D:153:VAL:CG2	1:D:173:ILE:HD13	2.06	0.77
1:D:93:TYR:HB3	1:D:96:ILE:HD13	1.67	0.77
1:A:89:PHE:O	1:A:90:PRO:O	2.03	0.76
1:A:259:MET:O	1:A:263:THR:HG23	1.86	0.76
1:A:136:ARG:HB3	1:A:315:LEU:HD11	1.68	0.75
1:D:219:ARG:NH1	1:D:302:GLU:OE2	2.19	0.75
1:C:219:ARG:NH1	1:C:302:GLU:OE2	2.19	0.75
1:A:95:GLU:HG2	1:A:96:ILE:HD12	1.69	0.75
1:B:219:ARG:NH1	1:B:302:GLU:OE2	2.19	0.74
1:A:153:VAL:HG22	1:A:173:ILE:CD1	2.14	0.73
1:B:298:LYS:O	1:B:302:GLU:HG3	1.87	0.73
1:A:298:LYS:O	1:A:302:GLU:HG3	1.87	0.73
1:C:28:LYS:HA	1:C:28:LYS:HE2	1.70	0.73
1:B:86:THR:O	1:B:88:LEU:HB2	1.88	0.73
1:C:89:PHE:O	1:C:90:PRO:O	2.05	0.73
1:A:219:ARG:NH1	1:A:302:GLU:OE2	2.21	0.73
1:A:28:LYS:HA	1:A:28:LYS:HE2	1.71	0.73
1:B:28:LYS:HE2	1:B:28:LYS:HA	1.70	0.73
1:B:259:MET:O	1:B:263:THR:HG23	1.88	0.72
1:A:345:LYS:H	1:A:345:LYS:HD2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:LYS:HE2	1:D:28:LYS:HA	1.70	0.72
1:D:45:LYS:HB2	1:D:309:ARG:HE	1.54	0.72
1:B:45:LYS:HB2	1:B:309:ARG:HE	1.55	0.72
1:C:298:LYS:O	1:C:302:GLU:HG3	1.90	0.72
1:B:122:TRP:O	1:B:131:ARG:HD3	1.90	0.72
1:D:292:ASP:HB3	1:D:295:ILE:CD1	2.20	0.71
1:C:45:LYS:CG	1:C:309:ARG:NH2	2.53	0.71
1:D:136:ARG:HB3	1:D:315:LEU:HD11	1.71	0.71
1:A:133:PHE:CE2	1:A:137:VAL:HG21	2.25	0.71
1:C:136:ARG:HB3	1:C:315:LEU:HD11	1.71	0.71
1:A:323:ASN:ND2	1:A:326:LEU:HG	2.06	0.71
1:D:298:LYS:O	1:D:302:GLU:HG3	1.90	0.71
1:B:323:ASN:ND2	1:B:326:LEU:HG	2.05	0.71
1:D:323:ASN:ND2	1:D:326:LEU:HG	2.05	0.70
1:D:150:GLU:O	1:D:154:GLU:HB2	1.91	0.70
1:A:48:LEU:O	1:A:51:ASP:HB2	1.91	0.70
1:A:156:PHE:O	1:A:159:GLU:O	2.10	0.70
1:C:78:LEU:HD11	1:C:286:HIS:HB2	1.74	0.70
1:B:292:ASP:HB3	1:B:295:ILE:CD1	2.20	0.70
1:D:48:LEU:O	1:D:51:ASP:HB2	1.92	0.70
1:A:78:LEU:HD11	1:A:286:HIS:HB2	1.74	0.70
1:D:140:PHE:HE1	1:D:207:ILE:CD1	2.05	0.69
1:C:45:LYS:HG2	1:C:309:ARG:NH2	2.07	0.69
1:B:136:ARG:HB3	1:B:315:LEU:HD11	1.73	0.69
1:A:87:VAL:HG11	1:A:90:PRO:HG2	1.74	0.69
1:C:323:ASN:ND2	1:C:326:LEU:HG	2.06	0.69
1:C:134:ILE:HA	1:C:137:VAL:HG12	1.74	0.69
1:C:48:LEU:O	1:C:51:ASP:HB2	1.93	0.69
1:A:122:TRP:O	1:A:131:ARG:HD3	1.93	0.69
1:D:78:LEU:HD11	1:D:286:HIS:HB2	1.73	0.69
1:D:302:GLU:O	1:D:306:ILE:HG13	1.93	0.68
1:C:302:GLU:O	1:C:306:ILE:HG13	1.93	0.68
1:A:292:ASP:HB3	1:A:295:ILE:CD1	2.19	0.68
1:C:292:ASP:HB3	1:C:295:ILE:CD1	2.20	0.68
1:C:113:ILE:HD12	1:C:264:PHE:CD2	2.28	0.68
1:A:169:TYR:O	1:A:173:ILE:HG13	1.93	0.68
1:D:95:GLU:CG	1:D:282:LEU:HD21	2.23	0.68
1:A:302:GLU:O	1:A:306:ILE:HG13	1.94	0.67
1:B:169:TYR:O	1:B:173:ILE:HG13	1.94	0.67
1:D:86:THR:O	1:D:88:LEU:HB2	1.95	0.67
1:A:295:ILE:N	1:A:295:ILE:HD12	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ILE:N	1:D:295:ILE:HD12	2.10	0.67
1:B:91:ILE:O	1:B:94:HIS:CE1	2.48	0.66
1:C:169:TYR:O	1:C:173:ILE:HG13	1.96	0.66
1:D:140:PHE:CE1	1:D:207:ILE:HD13	2.28	0.66
1:B:312:LEU:HD11	1:B:328:ASN:OD1	1.96	0.66
1:A:153:VAL:CG1	1:D:153:VAL:HG11	2.26	0.66
1:C:295:ILE:N	1:C:295:ILE:HD12	2.11	0.66
1:D:312:LEU:HD11	1:D:328:ASN:OD1	1.96	0.66
1:B:295:ILE:HD12	1:B:295:ILE:N	2.10	0.65
1:B:323:ASN:HB3	1:B:326:LEU:HD12	1.78	0.65
1:B:302:GLU:O	1:B:306:ILE:HG13	1.95	0.65
1:D:323:ASN:HB3	1:D:326:LEU:HD12	1.79	0.64
1:B:42:ASP:HA	1:B:45:LYS:HB3	1.78	0.64
1:C:312:LEU:HD11	1:C:328:ASN:OD1	1.97	0.64
1:C:323:ASN:HB3	1:C:326:LEU:HD12	1.80	0.64
1:A:312:LEU:HD11	1:A:328:ASN:OD1	1.98	0.64
1:C:113:ILE:HD12	1:C:264:PHE:HD2	1.61	0.64
1:C:140:PHE:CE1	1:C:310:TYR:CD2	2.86	0.64
1:D:169:TYR:O	1:D:173:ILE:HG13	1.97	0.64
1:C:117:LYS:HB2	1:C:260:PRO:HG3	1.80	0.63
1:B:323:ASN:HD22	1:B:326:LEU:CG	2.11	0.63
1:C:45:LYS:HG2	1:C:309:ARG:CZ	2.28	0.63
1:A:256:ARG:O	1:A:258:MET:HG3	1.98	0.63
1:A:45:LYS:HB2	1:A:309:ARG:NE	2.12	0.63
1:B:256:ARG:O	1:B:258:MET:HG3	1.99	0.63
1:D:91:ILE:O	1:D:94:HIS:CE1	2.51	0.63
1:A:323:ASN:HB3	1:A:326:LEU:HD12	1.80	0.62
1:C:122:TRP:O	1:C:131:ARG:HD3	1.98	0.62
1:A:323:ASN:HD22	1:A:326:LEU:CG	2.11	0.62
1:D:323:ASN:HD22	1:D:326:LEU:CG	2.11	0.62
1:B:48:LEU:HA	1:B:51:ASP:OD2	1.98	0.62
1:D:122:TRP:O	1:D:131:ARG:HD3	1.99	0.62
1:C:48:LEU:HA	1:C:51:ASP:OD2	1.99	0.62
1:D:211:GLY:O	1:D:214:ALA:HB3	2.00	0.62
1:B:153:VAL:CG1	1:C:153:VAL:HG11	2.30	0.62
1:D:95:GLU:HG3	1:D:282:LEU:HD11	1.81	0.62
1:B:153:VAL:CG1	1:C:153:VAL:CG1	2.77	0.61
1:D:284:PHE:O	1:D:287:LEU:HB2	2.00	0.61
1:C:211:GLY:O	1:C:214:ALA:HB3	2.01	0.61
1:D:326:LEU:HD22	1:D:353:PRO:HB2	1.83	0.61
1:C:284:PHE:O	1:C:287:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:O	1:B:51:ASP:CB	2.48	0.61
1:C:193:ASP:OD2	1:C:195:LYS:HB3	2.01	0.61
1:C:326:LEU:HD22	1:C:353:PRO:HB2	1.83	0.61
1:D:45:LYS:HB2	1:D:309:ARG:NE	2.15	0.61
1:C:45:LYS:HG3	1:C:309:ARG:NH2	2.16	0.61
1:C:323:ASN:HD22	1:C:326:LEU:CG	2.12	0.61
1:B:70:LYS:HE3	1:B:225:ASP:HA	1.83	0.60
1:D:351:GLU:O	1:D:353:PRO:HD3	2.01	0.60
1:C:256:ARG:O	1:C:258:MET:HG3	2.01	0.60
1:A:42:ASP:HA	1:A:45:LYS:HB3	1.84	0.60
1:D:42:ASP:HA	1:D:45:LYS:HB3	1.84	0.60
1:B:45:LYS:HG3	1:B:309:ARG:NH2	2.16	0.60
1:D:95:GLU:OE2	1:D:95:GLU:CA	2.48	0.60
1:C:351:GLU:O	1:C:353:PRO:HD3	2.02	0.59
1:C:140:PHE:CE1	1:C:310:TYR:HD2	2.20	0.59
1:B:193:ASP:OD2	1:B:195:LYS:HB3	2.02	0.59
1:C:116:SER:O	1:C:119:ILE:HG22	2.03	0.59
1:B:351:GLU:O	1:B:353:PRO:HD3	2.03	0.59
1:D:284:PHE:CZ	1:D:291:PRO:HD2	2.38	0.59
1:C:284:PHE:CZ	1:C:291:PRO:HD2	2.38	0.59
1:A:153:VAL:HG11	1:D:153:VAL:CG1	2.33	0.59
1:B:45:LYS:HB2	1:B:309:ARG:NE	2.18	0.59
1:C:96:ILE:HD12	1:C:96:ILE:N	2.17	0.59
1:A:153:VAL:CG1	1:D:153:VAL:CG1	2.80	0.59
1:B:284:PHE:CZ	1:B:291:PRO:HD2	2.38	0.59
1:A:96:ILE:HD12	1:A:96:ILE:N	2.17	0.58
1:A:284:PHE:O	1:A:287:LEU:HB2	2.03	0.58
1:B:211:GLY:O	1:B:214:ALA:HB3	2.02	0.58
1:D:256:ARG:O	1:D:258:MET:HG3	2.03	0.58
1:D:96:ILE:N	1:D:96:ILE:HD12	2.18	0.58
1:C:163:PRO:HG2	1:C:164:GLU:OE2	2.04	0.58
1:A:351:GLU:O	1:A:353:PRO:HD3	2.04	0.58
1:C:95:GLU:HG2	1:C:96:ILE:HD12	1.86	0.58
1:B:304:VAL:O	1:B:308:GLN:HG3	2.04	0.58
1:A:211:GLY:O	1:A:214:ALA:HB3	2.04	0.58
1:B:326:LEU:HD22	1:B:353:PRO:HB2	1.86	0.57
1:A:84:GLU:O	1:A:84:GLU:HG2	2.04	0.57
1:A:163:PRO:HG2	1:A:164:GLU:OE2	2.05	0.57
1:A:193:ASP:OD2	1:A:195:LYS:HB3	2.04	0.57
1:A:48:LEU:HA	1:A:51:ASP:OD2	2.04	0.57
1:A:326:LEU:HD22	1:A:353:PRO:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:HE2	1:A:137:VAL:HG21	1.67	0.57
1:B:284:PHE:O	1:B:287:LEU:HB2	2.04	0.57
1:A:152:LEU:HD21	1:A:169:TYR:HD1	1.70	0.57
1:B:153:VAL:HG11	1:C:153:VAL:CG1	2.35	0.57
1:A:304:VAL:O	1:A:308:GLN:HG3	2.05	0.57
1:A:284:PHE:CZ	1:A:291:PRO:HD2	2.39	0.57
1:C:155:ASN:ND2	1:C:231:ARG:HD2	2.20	0.56
1:B:218:LEU:HA	1:B:222:GLN:HB2	1.86	0.56
1:C:307:GLU:O	1:C:310:TYR:HB2	2.06	0.56
1:A:70:LYS:HE3	1:A:225:ASP:HA	1.88	0.56
1:B:84:GLU:HG2	1:B:84:GLU:O	2.05	0.56
1:C:118:ASP:OD1	1:C:260:PRO:HG2	2.04	0.56
1:C:84:GLU:O	1:C:84:GLU:HG2	2.05	0.56
1:D:155:ASN:HD21	1:D:231:ARG:CD	2.12	0.56
1:B:78:LEU:CD2	1:B:283:LEU:HD22	2.25	0.56
1:A:118:ASP:OD1	1:A:260:PRO:HG2	2.06	0.56
1:C:304:VAL:O	1:C:308:GLN:HG3	2.06	0.56
1:A:152:LEU:HD13	1:A:173:ILE:HG12	1.87	0.55
1:D:84:GLU:HG2	1:D:84:GLU:O	2.05	0.55
1:A:155:ASN:ND2	1:A:231:ARG:HD2	2.21	0.55
1:B:304:VAL:HG13	1:B:331:VAL:HG12	1.89	0.55
1:A:207:ILE:HG22	1:A:209:GLU:OE1	2.05	0.55
1:D:304:VAL:O	1:D:308:GLN:HG3	2.07	0.55
1:A:218:LEU:HA	1:A:222:GLN:HB2	1.87	0.55
1:D:307:GLU:O	1:D:310:TYR:HB2	2.05	0.55
1:B:87:VAL:HG22	1:B:90:PRO:HD2	1.88	0.55
1:D:97:TRP:O	1:D:100:TYR:N	2.39	0.55
1:C:32:THR:O	1:C:36:GLU:HG3	2.05	0.55
1:C:97:TRP:O	1:C:100:TYR:N	2.39	0.55
1:B:207:ILE:HG22	1:B:209:GLU:OE1	2.07	0.55
1:B:137:VAL:HG23	1:B:315:LEU:CD1	2.37	0.55
1:C:87:VAL:HG11	1:C:90:PRO:HG2	1.89	0.55
1:B:118:ASP:OD1	1:B:260:PRO:HG2	2.06	0.55
1:B:163:PRO:HG2	1:B:164:GLU:OE2	2.07	0.55
1:A:152:LEU:HD21	1:A:169:TYR:CD1	2.41	0.54
1:D:295:ILE:H	1:D:295:ILE:HD12	1.72	0.54
1:B:153:VAL:HG22	1:B:173:ILE:CD1	2.23	0.54
1:C:207:ILE:HG22	1:C:209:GLU:OE1	2.06	0.54
1:A:117:LYS:HB3	1:A:260:PRO:HG3	1.89	0.54
1:B:117:LYS:HB3	1:B:260:PRO:HG3	1.89	0.54
1:D:32:THR:O	1:D:35:GLU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD23	1:A:218:LEU:O	2.08	0.54
1:D:32:THR:O	1:D:36:GLU:HG3	2.07	0.54
1:D:207:ILE:HG22	1:D:209:GLU:OE1	2.07	0.54
1:A:130:GLU:OE1	1:A:256:ARG:NH2	2.40	0.54
1:C:218:LEU:HA	1:C:222:GLN:HB2	1.89	0.54
1:D:70:LYS:HE3	1:D:225:ASP:HA	1.90	0.54
1:A:32:THR:O	1:A:36:GLU:HG3	2.08	0.54
1:C:304:VAL:HG13	1:C:331:VAL:HG12	1.90	0.54
1:A:137:VAL:HG23	1:A:315:LEU:CD1	2.38	0.53
1:B:32:THR:O	1:B:35:GLU:HB3	2.07	0.53
1:C:70:LYS:HE3	1:C:225:ASP:HA	1.89	0.53
1:A:32:THR:O	1:A:35:GLU:HB3	2.07	0.53
1:B:130:GLU:OE1	1:B:256:ARG:NH2	2.41	0.53
1:D:218:LEU:HA	1:D:222:GLN:HB2	1.89	0.53
1:C:295:ILE:H	1:C:295:ILE:HD12	1.72	0.53
1:A:307:GLU:O	1:A:310:TYR:HB2	2.09	0.53
1:D:304:VAL:HG13	1:D:331:VAL:HG12	1.89	0.53
1:C:96:ILE:O	1:C:99:ALA:N	2.42	0.53
1:B:97:TRP:O	1:B:100:TYR:N	2.42	0.53
1:C:32:THR:O	1:C:35:GLU:HB3	2.08	0.53
1:D:194:PRO:HA	1:D:197:SER:HB3	1.91	0.53
1:C:194:PRO:HA	1:C:197:SER:HB3	1.91	0.53
1:D:130:GLU:OE1	1:D:256:ARG:NH2	2.42	0.53
1:A:97:TRP:O	1:A:100:TYR:N	2.42	0.53
1:A:96:ILE:O	1:A:99:ALA:N	2.42	0.52
1:A:140:PHE:CE1	1:A:207:ILE:HD13	2.44	0.52
1:D:155:ASN:O	1:D:159:GLU:OE1	2.27	0.52
1:A:317:VAL:HB	1:A:322:MET:CB	2.37	0.52
1:C:204:ILE:O	1:C:210:ILE:HD11	2.09	0.52
1:B:32:THR:O	1:B:36:GLU:HG3	2.09	0.52
1:B:194:PRO:HA	1:B:197:SER:HB3	1.92	0.52
1:C:130:GLU:OE1	1:C:256:ARG:NH2	2.42	0.52
1:B:307:GLU:O	1:B:310:TYR:HB2	2.08	0.52
1:B:218:LEU:HD23	1:B:218:LEU:O	2.09	0.52
1:B:295:ILE:HD12	1:B:295:ILE:H	1.73	0.52
1:C:42:ASP:HA	1:C:45:LYS:HB2	1.90	0.52
1:A:155:ASN:HD21	1:A:231:ARG:HD2	1.75	0.52
1:B:58:TYR:O	1:B:62:HIS:HD2	1.93	0.52
1:D:218:LEU:HD23	1:D:218:LEU:O	2.10	0.52
1:A:34:ARG:NE	1:A:313:ASP:O	2.43	0.52
1:A:58:TYR:O	1:A:62:HIS:HD2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:PHE:CE2	1:D:290:LYS:HD3	2.45	0.52
1:A:116:SER:O	1:A:119:ILE:HG22	2.10	0.52
1:A:81:GLU:HG3	1:A:161:GLN:NE2	2.25	0.52
1:C:45:LYS:HG3	1:C:309:ARG:HH21	1.73	0.51
1:C:34:ARG:NE	1:C:313:ASP:O	2.42	0.51
1:A:269:ILE:O	1:A:272:ASP:HB2	2.10	0.51
1:D:204:ILE:O	1:D:210:ILE:HD11	2.10	0.51
1:D:96:ILE:O	1:D:99:ALA:N	2.42	0.51
1:B:220:TRP:CD2	1:B:299:ILE:HG12	2.45	0.51
1:A:204:ILE:O	1:A:210:ILE:HD11	2.11	0.51
1:A:304:VAL:HG13	1:A:331:VAL:HG12	1.90	0.51
1:D:137:VAL:HG23	1:D:315:LEU:CD1	2.41	0.51
1:D:34:ARG:NE	1:D:313:ASP:O	2.42	0.51
1:A:87:VAL:CG2	1:A:90:PRO:HD2	2.41	0.51
1:D:95:GLU:HG3	1:D:282:LEU:CD2	2.36	0.51
1:C:45:LYS:CG	1:C:309:ARG:HH21	2.24	0.51
1:A:194:PRO:HA	1:A:197:SER:HB3	1.91	0.51
1:D:220:TRP:CD2	1:D:299:ILE:HG12	2.46	0.51
1:A:295:ILE:H	1:A:295:ILE:HD12	1.72	0.51
1:C:284:PHE:CE2	1:C:290:LYS:HD3	2.46	0.51
1:C:220:TRP:CD2	1:C:299:ILE:HG12	2.46	0.51
1:D:317:VAL:HB	1:D:322:MET:CB	2.38	0.50
1:B:34:ARG:NE	1:B:313:ASP:O	2.44	0.50
1:D:116:SER:O	1:D:119:ILE:HG22	2.11	0.50
1:B:45:LYS:CG	1:B:309:ARG:NH2	2.74	0.50
1:D:172:GLN:HG3	1:D:276:HIS:CD2	2.47	0.50
1:A:140:PHE:HE1	1:A:207:ILE:HD13	1.75	0.50
1:D:96:ILE:H	1:D:96:ILE:HD12	1.76	0.50
1:B:204:ILE:O	1:B:210:ILE:HD11	2.12	0.50
1:C:96:ILE:HD12	1:C:96:ILE:H	1.76	0.50
1:A:96:ILE:H	1:A:96:ILE:HD12	1.76	0.50
1:B:131:ARG:HG3	1:B:131:ARG:HH11	1.77	0.50
1:A:28:LYS:HE2	1:A:28:LYS:CA	2.42	0.49
1:C:332:GLU:HG2	1:C:348:TYR:CE2	2.47	0.49
1:D:345:LYS:HD2	1:D:345:LYS:H	1.78	0.49
1:A:45:LYS:HG3	1:A:309:ARG:NH2	2.28	0.49
1:A:172:GLN:HG3	1:A:276:HIS:NE2	2.27	0.49
1:D:48:LEU:HA	1:D:51:ASP:OD2	2.11	0.49
1:A:172:GLN:HG3	1:A:276:HIS:CD2	2.48	0.49
1:C:113:ILE:HD13	1:C:113:ILE:N	2.26	0.49
1:D:332:GLU:HG2	1:D:348:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLN:HG3	1:C:276:HIS:CD2	2.48	0.49
1:C:134:ILE:HA	1:C:137:VAL:CG1	2.41	0.49
1:C:218:LEU:HD23	1:C:218:LEU:O	2.12	0.49
1:B:81:GLU:HG3	1:B:161:GLN:NE2	2.28	0.49
1:B:116:SER:O	1:B:119:ILE:HG22	2.11	0.49
1:A:49:SER:O	1:A:51:ASP:N	2.42	0.49
1:B:183:TYR:OH	1:B:269:ILE:HG21	2.13	0.49
1:A:183:TYR:OH	1:A:269:ILE:HG21	2.13	0.49
1:D:268:LEU:HD22	1:D:271:ARG:HH21	1.77	0.49
1:C:234:ALA:O	1:C:238:ILE:HG13	2.13	0.49
1:D:311:PHE:HD2	1:D:315:LEU:O	1.95	0.48
1:A:268:LEU:HD22	1:A:271:ARG:HH21	1.78	0.48
1:D:234:ALA:O	1:D:238:ILE:HG13	2.13	0.48
1:A:82:ASP:O	1:A:84:GLU:N	2.47	0.48
1:A:332:GLU:HG2	1:A:348:TYR:CE2	2.48	0.48
1:A:295:ILE:H	1:A:295:ILE:CD1	2.27	0.48
1:D:356:PHE:CE1	1:D:357:MET:HG2	2.49	0.48
1:D:53:GLU:OE2	1:D:53:GLU:HA	2.13	0.48
1:C:129:ASN:HB3	1:C:319:LEU:O	2.13	0.48
1:C:295:ILE:H	1:C:295:ILE:CD1	2.27	0.48
1:D:258:MET:O	1:D:259:MET:C	2.51	0.48
1:A:125:ARG:HB3	1:A:258:MET:HE3	1.95	0.48
1:B:234:ALA:O	1:B:238:ILE:HG13	2.14	0.48
1:A:220:TRP:CD2	1:A:299:ILE:HG12	2.47	0.48
1:C:78:LEU:O	1:C:160:VAL:HA	2.14	0.48
1:B:284:PHE:CE2	1:B:290:LYS:HD3	2.48	0.48
1:B:269:ILE:O	1:B:272:ASP:HB2	2.12	0.48
1:C:81:GLU:HG3	1:C:161:GLN:NE2	2.27	0.48
1:A:132:PHE:O	1:A:133:PHE:C	2.51	0.48
1:B:53:GLU:HA	1:B:53:GLU:OE2	2.14	0.48
1:A:95:GLU:HG2	1:A:96:ILE:CD1	2.40	0.48
1:C:152:LEU:HD11	1:C:235:PHE:CE1	2.49	0.48
1:C:209:GLU:HG2	1:C:310:TYR:HA	1.94	0.48
1:B:311:PHE:HD2	1:B:315:LEU:O	1.97	0.48
1:B:268:LEU:HD22	1:B:271:ARG:HH21	1.79	0.48
1:C:356:PHE:CE1	1:C:357:MET:HG2	2.49	0.48
1:A:300:VAL:O	1:A:304:VAL:HG23	2.14	0.47
1:D:129:ASN:HB3	1:D:319:LEU:O	2.13	0.47
1:C:53:GLU:OE2	1:C:53:GLU:HA	2.13	0.47
1:D:295:ILE:CD1	1:D:295:ILE:N	2.76	0.47
1:D:209:GLU:HG2	1:D:310:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:O	1:B:84:GLU:N	2.47	0.47
1:D:295:ILE:CD1	1:D:295:ILE:H	2.26	0.47
1:C:140:PHE:CE1	1:C:310:TYR:CE2	3.03	0.47
1:B:125:ARG:HB3	1:B:258:MET:HE3	1.96	0.47
1:B:172:GLN:HG3	1:B:276:HIS:CD2	2.49	0.47
1:A:209:GLU:HG2	1:A:310:TYR:HA	1.97	0.47
1:C:311:PHE:HD2	1:C:315:LEU:O	1.97	0.47
1:A:295:ILE:N	1:A:295:ILE:CD1	2.76	0.47
1:A:311:PHE:HD2	1:A:315:LEU:O	1.98	0.47
1:B:28:LYS:CA	1:B:28:LYS:HE2	2.42	0.47
1:B:155:ASN:ND2	1:B:231:ARG:HD2	2.30	0.47
1:A:53:GLU:HA	1:A:53:GLU:OE2	2.15	0.47
1:C:268:LEU:HD22	1:C:271:ARG:HH21	1.78	0.47
1:D:197:SER:O	1:D:201:PHE:HD1	1.98	0.47
1:D:78:LEU:O	1:D:160:VAL:HA	2.14	0.47
1:B:300:VAL:O	1:B:304:VAL:HG23	2.15	0.47
1:D:329:GLN:NE2	1:D:353:PRO:HB3	2.30	0.46
1:B:129:ASN:HB3	1:B:319:LEU:O	2.14	0.46
1:D:204:ILE:O	1:D:207:ILE:HD12	2.16	0.46
1:B:172:GLN:HG3	1:B:276:HIS:NE2	2.30	0.46
1:A:140:PHE:HE1	1:A:207:ILE:CD1	2.29	0.46
1:C:295:ILE:N	1:C:295:ILE:CD1	2.77	0.46
1:C:300:VAL:O	1:C:303:ALA:HB3	2.14	0.46
1:A:129:ASN:HB3	1:A:319:LEU:O	2.15	0.46
1:D:125:ARG:HB3	1:D:258:MET:HE3	1.97	0.46
1:D:270:CYS:O	1:D:271:ARG:C	2.54	0.46
1:A:83:LYS:HB2	1:A:83:LYS:HE3	1.78	0.46
1:D:82:ASP:O	1:D:84:GLU:N	2.49	0.46
1:A:172:GLN:HG3	1:A:276:HIS:CE1	2.51	0.46
1:B:295:ILE:CD1	1:B:295:ILE:H	2.28	0.46
1:D:269:ILE:O	1:D:272:ASP:HB2	2.16	0.46
1:C:329:GLN:NE2	1:C:353:PRO:HB3	2.31	0.46
1:D:96:ILE:O	1:D:99:ALA:HB3	2.16	0.46
1:D:300:VAL:O	1:D:303:ALA:HB3	2.15	0.46
1:C:197:SER:O	1:C:201:PHE:HD1	1.98	0.46
1:C:118:ASP:OD1	1:C:261:GLY:N	2.39	0.46
1:B:295:ILE:N	1:B:295:ILE:CD1	2.76	0.46
1:D:300:VAL:O	1:D:304:VAL:HG23	2.16	0.46
1:C:300:VAL:O	1:C:304:VAL:HG23	2.16	0.46
1:A:284:PHE:CE2	1:A:290:LYS:HD3	2.51	0.46
1:D:69:LEU:HA	1:D:72:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:MET:HG2	1:C:258:MET:HE1	1.98	0.45
1:C:82:ASP:O	1:C:84:GLU:N	2.49	0.45
1:A:197:SER:O	1:A:201:PHE:HD1	2.00	0.45
1:B:197:SER:O	1:B:201:PHE:HD1	2.00	0.45
1:D:69:LEU:HD23	1:D:72:MET:CE	2.46	0.45
1:A:345:LYS:CD	1:A:345:LYS:H	2.28	0.45
1:C:204:ILE:O	1:C:207:ILE:HD12	2.16	0.45
1:A:87:VAL:HG22	1:A:90:PRO:HD2	1.98	0.45
1:B:155:ASN:HD21	1:B:231:ARG:HD2	1.82	0.45
1:B:156:PHE:CE2	1:B:232:LEU:HD23	2.52	0.45
1:C:96:ILE:O	1:C:99:ALA:HB3	2.16	0.45
1:C:28:LYS:CA	1:C:28:LYS:HE2	2.41	0.45
1:A:133:PHE:HZ	1:A:249:SER:HB2	1.82	0.45
1:A:270:CYS:O	1:A:271:ARG:C	2.53	0.45
1:B:140:PHE:O	1:B:141:PHE:C	2.55	0.45
1:A:91:ILE:O	1:A:94:HIS:CE1	2.69	0.45
1:A:234:ALA:O	1:A:238:ILE:HG13	2.16	0.45
1:A:96:ILE:O	1:A:99:ALA:HB3	2.17	0.45
1:B:209:GLU:HG2	1:B:310:TYR:HA	1.98	0.45
1:D:172:GLN:HG3	1:D:276:HIS:NE2	2.32	0.45
1:C:317:VAL:HB	1:C:322:MET:CB	2.38	0.45
1:D:96:ILE:H	1:D:96:ILE:CD1	2.30	0.45
1:B:83:LYS:HE3	1:B:83:LYS:HB2	1.77	0.45
1:B:172:GLN:HG3	1:B:276:HIS:CE1	2.52	0.44
1:C:168:PHE:C	1:C:168:PHE:CD1	2.91	0.44
1:C:69:LEU:HD23	1:C:72:MET:CE	2.46	0.44
1:C:172:GLN:HG3	1:C:276:HIS:NE2	2.33	0.44
1:C:69:LEU:HA	1:C:72:MET:CE	2.47	0.44
1:D:168:PHE:CD1	1:D:168:PHE:C	2.91	0.44
1:D:118:ASP:OD1	1:D:260:PRO:HG2	2.17	0.44
1:D:73:GLU:C	1:D:75:GLU:H	2.21	0.44
1:D:28:LYS:HE2	1:D:28:LYS:CA	2.41	0.44
1:B:300:VAL:O	1:B:303:ALA:HB3	2.18	0.44
1:B:270:CYS:O	1:B:271:ARG:C	2.52	0.44
1:D:156:PHE:CE2	1:D:232:LEU:HD23	2.52	0.44
1:C:183:TYR:OH	1:C:269:ILE:HG21	2.18	0.44
1:B:168:PHE:CD1	1:B:168:PHE:C	2.91	0.44
1:C:96:ILE:H	1:C:96:ILE:CD1	2.30	0.44
1:A:96:ILE:H	1:A:96:ILE:CD1	2.30	0.44
1:C:270:CYS:O	1:C:271:ARG:C	2.54	0.44
1:D:183:TYR:OH	1:D:269:ILE:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:CG	1:A:309:ARG:NH2	2.81	0.44
1:A:168:PHE:CD1	1:A:168:PHE:C	2.91	0.44
1:B:53:GLU:O	1:B:55:HIS:N	2.51	0.44
1:A:356:PHE:CE1	1:A:357:MET:HG2	2.53	0.44
1:A:152:LEU:HD11	1:A:172:GLN:NE2	2.33	0.44
1:D:204:ILE:O	1:D:207:ILE:CD1	2.66	0.44
1:A:209:GLU:OE2	1:A:309:ARG:NH1	2.50	0.44
1:C:193:ASP:O	1:C:196:GLU:N	2.50	0.44
1:B:356:PHE:CE1	1:B:357:MET:HG2	2.53	0.44
1:B:26:LEU:C	1:B:28:LYS:N	2.72	0.43
1:B:193:ASP:OD2	1:B:195:LYS:HE2	2.17	0.43
1:D:252:TRP:CZ3	1:D:255:LYS:HE3	2.53	0.43
1:B:69:LEU:HD23	1:B:72:MET:CE	2.48	0.43
1:D:209:GLU:OE2	1:D:309:ARG:NH1	2.51	0.43
1:D:45:LYS:HG3	1:D:309:ARG:NH2	2.34	0.43
1:A:204:ILE:O	1:A:207:ILE:CD1	2.67	0.43
1:D:96:ILE:O	1:D:97:TRP:C	2.56	0.43
1:D:131:ARG:HH11	1:D:131:ARG:HG3	1.82	0.43
1:C:155:ASN:HD21	1:C:231:ARG:HD2	1.82	0.43
1:D:358:GLU:O	1:D:359:ASN:HB2	2.18	0.43
1:C:87:VAL:HG22	1:C:90:PRO:HD2	1.99	0.43
1:A:117:LYS:NZ	1:A:121:ASP:OD2	2.52	0.43
1:B:53:GLU:C	1:B:55:HIS:N	2.71	0.43
1:A:162:ILE:HG13	1:A:162:ILE:O	2.18	0.43
1:C:258:MET:O	1:C:259:MET:C	2.56	0.43
1:A:300:VAL:O	1:A:303:ALA:HB3	2.18	0.43
1:D:332:GLU:HG2	1:D:348:TYR:CD2	2.54	0.43
1:A:53:GLU:O	1:A:55:HIS:N	2.51	0.43
1:C:252:TRP:CZ3	1:C:255:LYS:HE3	2.53	0.43
1:B:73:GLU:C	1:B:75:GLU:H	2.22	0.43
1:A:204:ILE:O	1:A:207:ILE:HD12	2.18	0.43
1:A:117:LYS:NZ	1:A:125:ARG:HH11	2.17	0.43
1:B:117:LYS:NZ	1:B:125:ARG:HH11	2.17	0.43
1:C:209:GLU:OE2	1:C:309:ARG:NH1	2.52	0.43
1:B:70:LYS:O	1:B:70:LYS:HG3	2.19	0.43
1:B:69:LEU:HA	1:B:72:MET:CE	2.49	0.43
1:B:177:ASN:HD22	1:B:177:ASN:HA	1.70	0.43
1:C:204:ILE:O	1:C:207:ILE:CD1	2.66	0.43
1:C:150:GLU:HG3	1:C:154:GLU:OE2	2.19	0.43
1:D:87:VAL:HG23	1:D:90:PRO:HG2	1.99	0.43
1:A:96:ILE:N	1:A:96:ILE:CD1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:O	1:C:272:ASP:HB2	2.17	0.43
1:B:153:VAL:HG13	1:C:153:VAL:HG11	2.01	0.43
1:C:96:ILE:CD1	1:C:96:ILE:N	2.81	0.43
1:B:204:ILE:O	1:B:207:ILE:HD12	2.19	0.43
1:B:127:ASN:O	1:B:131:ARG:NH1	2.52	0.43
1:C:69:LEU:HA	1:C:72:MET:HE2	2.00	0.43
1:B:209:GLU:OE2	1:B:309:ARG:NH1	2.52	0.42
1:D:356:PHE:CD1	1:D:357:MET:HG2	2.54	0.42
1:C:96:ILE:O	1:C:97:TRP:C	2.56	0.42
1:A:26:LEU:C	1:A:28:LYS:N	2.72	0.42
1:C:356:PHE:CD1	1:C:357:MET:HG2	2.54	0.42
1:A:73:GLU:C	1:A:75:GLU:H	2.22	0.42
1:C:193:ASP:OD2	1:C:195:LYS:HE2	2.19	0.42
1:A:53:GLU:C	1:A:55:HIS:N	2.71	0.42
1:D:232:LEU:HA	1:D:232:LEU:HD23	1.91	0.42
1:A:308:GLN:HB3	1:A:328:ASN:ND2	2.35	0.42
1:B:252:TRP:CZ3	1:B:255:LYS:HE3	2.55	0.42
1:B:204:ILE:O	1:B:207:ILE:CD1	2.68	0.42
1:C:308:GLN:HB3	1:C:328:ASN:ND2	2.35	0.42
1:A:78:LEU:O	1:A:160:VAL:HA	2.20	0.42
1:D:162:ILE:HG13	1:D:165:ALA:HB3	2.02	0.42
1:B:87:VAL:CG2	1:B:90:PRO:HD2	2.49	0.42
1:B:117:LYS:NZ	1:B:121:ASP:OD2	2.51	0.42
1:C:53:GLU:C	1:C:55:HIS:N	2.73	0.42
1:C:83:LYS:C	1:C:85:ARG:H	2.23	0.42
1:D:209:GLU:HB3	1:D:310:TYR:CE1	2.55	0.42
1:C:162:ILE:HG13	1:C:162:ILE:O	2.20	0.42
1:B:127:ASN:C	1:B:131:ARG:NH1	2.73	0.42
1:C:209:GLU:HB3	1:C:310:TYR:CE1	2.55	0.42
1:C:113:ILE:HA	1:C:113:ILE:HD12	1.90	0.42
1:B:69:LEU:HA	1:B:72:MET:HE3	2.00	0.42
1:C:83:LYS:HE3	1:C:83:LYS:HB2	1.79	0.42
1:D:50:LYS:HE2	1:D:50:LYS:HB3	1.85	0.42
1:B:49:SER:O	1:B:51:ASP:N	2.49	0.41
1:A:220:TRP:HZ2	1:A:302:GLU:OE1	2.03	0.41
1:D:26:LEU:C	1:D:28:LYS:N	2.73	0.41
1:D:316:PRO:HD2	1:D:319:LEU:HD12	2.01	0.41
1:B:258:MET:O	1:B:259:MET:C	2.58	0.41
1:B:308:GLN:HB3	1:B:328:ASN:ND2	2.35	0.41
1:C:328:ASN:HD22	1:C:328:ASN:HA	1.70	0.41
1:B:284:PHE:HZ	1:B:291:PRO:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLU:HG2	1:A:348:TYR:CD2	2.55	0.41
1:C:316:PRO:HD2	1:C:319:LEU:HD12	2.01	0.41
1:A:83:LYS:C	1:A:85:ARG:H	2.24	0.41
1:A:127:ASN:OD1	1:A:129:ASN:N	2.53	0.41
1:A:316:PRO:HD2	1:A:319:LEU:HD12	2.02	0.41
1:B:297:GLU:O	1:B:301:THR:HB	2.20	0.41
1:D:201:PHE:O	1:D:204:ILE:HG22	2.21	0.41
1:B:140:PHE:HE2	1:B:204:ILE:HD11	1.86	0.41
1:B:49:SER:C	1:B:51:ASP:H	2.24	0.41
1:C:220:TRP:HZ2	1:C:302:GLU:OE1	2.04	0.41
1:A:96:ILE:HG23	1:A:279:PHE:HE1	1.85	0.41
1:A:193:ASP:HA	1:A:194:PRO:HD2	1.92	0.41
1:D:308:GLN:HB3	1:D:328:ASN:ND2	2.35	0.41
1:A:70:LYS:HG3	1:A:70:LYS:O	2.19	0.41
1:B:55:HIS:O	1:B:56:LYS:C	2.58	0.41
1:D:193:ASP:OD1	1:D:195:LYS:HB2	2.21	0.41
1:A:193:ASP:OD2	1:A:195:LYS:HE2	2.20	0.41
1:B:176:GLU:OE1	1:B:273:GLU:OE1	2.39	0.41
1:A:69:LEU:HD23	1:A:72:MET:CE	2.50	0.41
1:C:73:GLU:C	1:C:75:GLU:H	2.22	0.41
1:D:140:PHE:O	1:D:141:PHE:C	2.59	0.41
1:B:317:VAL:HB	1:B:322:MET:CB	2.38	0.41
1:A:201:PHE:O	1:A:204:ILE:HG22	2.21	0.41
1:A:209:GLU:HB3	1:A:310:TYR:CE1	2.55	0.41
1:A:258:MET:O	1:A:259:MET:C	2.59	0.41
1:C:26:LEU:C	1:C:28:LYS:N	2.73	0.41
1:B:209:GLU:HB3	1:B:310:TYR:CE1	2.56	0.41
1:A:55:HIS:O	1:A:56:LYS:C	2.59	0.41
1:A:96:ILE:O	1:A:97:TRP:C	2.59	0.41
1:B:127:ASN:OD1	1:B:129:ASN:N	2.54	0.41
1:C:140:PHE:O	1:C:141:PHE:C	2.59	0.41
1:C:201:PHE:O	1:C:204:ILE:HG22	2.21	0.41
1:C:332:GLU:HG2	1:C:348:TYR:CD2	2.56	0.41
1:C:127:ASN:OD1	1:C:129:ASN:N	2.54	0.41
1:A:69:LEU:HA	1:A:72:MET:CE	2.51	0.41
1:A:297:GLU:O	1:A:301:THR:HB	2.20	0.41
1:C:76:GLU:OE1	1:C:288:LYS:HB2	2.21	0.41
1:B:76:GLU:OE1	1:B:288:LYS:HB2	2.20	0.41
1:A:152:LEU:CD2	1:A:169:TYR:CD1	3.03	0.41
1:A:69:LEU:HA	1:A:72:MET:HE2	2.03	0.41
1:B:96:ILE:HD12	1:B:96:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PHE:CE2	1:B:204:ILE:HD11	2.55	0.40
1:C:193:ASP:HA	1:C:194:PRO:HD2	1.93	0.40
1:D:283:LEU:HA	1:D:283:LEU:HD23	1.91	0.40
1:C:284:PHE:HZ	1:C:291:PRO:HD2	1.84	0.40
1:A:155:ASN:HD21	1:A:231:ARG:CD	2.34	0.40
1:D:53:GLU:C	1:D:55:HIS:N	2.73	0.40
1:A:117:LYS:HZ2	1:A:125:ARG:HH11	1.69	0.40
1:A:76:GLU:OE1	1:A:288:LYS:HB2	2.21	0.40
1:C:355:ASP:O	1:C:358:GLU:HG2	2.22	0.40
1:D:297:GLU:O	1:D:301:THR:HB	2.21	0.40
1:C:53:GLU:O	1:C:55:HIS:N	2.55	0.40
1:B:83:LYS:C	1:B:85:ARG:H	2.24	0.40
1:D:213:LYS:O	1:D:216:TRP:HB3	2.22	0.40
1:B:78:LEU:O	1:B:160:VAL:HA	2.21	0.40
1:D:323:ASN:HD21	1:D:325:ASP:HB2	1.87	0.40
1:A:193:ASP:O	1:A:196:GLU:N	2.51	0.40
1:B:316:PRO:HD2	1:B:319:LEU:HD12	2.03	0.40
1:C:297:GLU:O	1:C:301:THR:HB	2.21	0.40

All (3) 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:198:GLU:CD	1:C:95:GLU:OE2[1_445]	1.41	0.79
1:A:198:GLU:OE1	1:C:95:GLU:OE2[1_445]	1.46	0.74
1:A:198:GLU:OE2	1:C:95:GLU:OE2[1_445]	1.82	0.38

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	325/399 (82%)	277 (85%)	40 (12%)	8 (2%)	7 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	325/399 (82%)	275 (85%)	41 (13%)	9 (3%)	6 30
1	C	312/399 (78%)	265 (85%)	38 (12%)	9 (3%)	6 29
1	D	312/399 (78%)	267 (86%)	36 (12%)	9 (3%)	6 29
All	All	1274/1596 (80%)	1084 (85%)	155 (12%)	35 (3%)	6 31

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	90	PRO
1	D	90	PRO
1	A	83	LYS
1	A	89	PHE
1	A	90	PRO
1	A	257	GLY
1	B	83	LYS
1	B	87	VAL
1	B	89	PHE
1	B	90	PRO
1	B	257	GLY
1	C	83	LYS
1	C	87	VAL
1	C	89	PHE
1	C	257	GLY
1	D	83	LYS
1	D	89	PHE
1	D	257	GLY
1	A	160	VAL
1	A	319	LEU
1	B	319	LEU
1	C	160	VAL
1	C	242	PHE
1	D	160	VAL
1	D	344	ASN
1	A	74	LYS
1	B	160	VAL
1	B	242	PHE
1	C	344	ASN
1	D	242	PHE
1	C	352	ASN
1	D	352	ASN
1	B	352	ASN

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Mol	Chain	Res	Type
1	A	352	ASN
1	D	87	VAL

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	292/350 (83%)	273 (94%)	19 (6%)	21	57
1	B	292/350 (83%)	271 (93%)	21 (7%)	18	53
1	C	281/350 (80%)	258 (92%)	23 (8%)	14	47
1	D	281/350 (80%)	261 (93%)	20 (7%)	18	54
All	All	1146/1400 (82%)	1063 (93%)	83 (7%)	18	53

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	88	LEU
1	A	118	ASP
1	A	136	ARG
1	A	152	LEU
1	A	175	ILE
1	A	186	LEU
1	A	200	LEU
1	A	242	PHE
1	A	243	PHE
1	A	282	LEU
1	A	287	LEU
1	A	301	THR
1	A	310	TYR
1	A	317	VAL
1	A	320	LEU
1	A	336	ASP
1	A	339	LEU
1	A	345	LYS

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Mol	Chain	Res	Type
1	B	78	LEU
1	B	88	LEU
1	B	118	ASP
1	B	136	ARG
1	B	175	ILE
1	B	186	LEU
1	B	196	GLU
1	B	200	LEU
1	B	205	HIS
1	B	225	ASP
1	B	242	PHE
1	B	243	PHE
1	B	282	LEU
1	B	287	LEU
1	B	301	THR
1	B	310	TYR
1	B	317	VAL
1	B	320	LEU
1	B	336	ASP
1	B	339	LEU
1	B	345	LYS
1	C	45	LYS
1	C	46	GLU
1	C	49	SER
1	C	54	ASN
1	C	75	GLU
1	C	88	LEU
1	C	89	PHE
1	C	113	ILE
1	C	117	LYS
1	C	136	ARG
1	C	175	ILE
1	C	186	LEU
1	C	200	LEU
1	C	242	PHE
1	C	243	PHE
1	C	282	LEU
1	C	287	LEU
1	C	301	THR
1	C	310	TYR
1	C	317	VAL
1	C	320	LEU

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Mol	Chain	Res	Type
1	C	336	ASP
1	C	339	LEU
1	D	43	MET
1	D	54	ASN
1	D	88	LEU
1	D	118	ASP
1	D	136	ARG
1	D	175	ILE
1	D	186	LEU
1	D	200	LEU
1	D	242	PHE
1	D	243	PHE
1	D	282	LEU
1	D	287	LEU
1	D	288	LYS
1	D	301	THR
1	D	310	TYR
1	D	317	VAL
1	D	320	LEU
1	D	336	ASP
1	D	339	LEU
1	D	345	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	129	ASN
1	A	151	ASN
1	A	155	ASN
1	A	161	GLN
1	A	172	GLN
1	A	177	ASN
1	A	202	ASN
1	A	205	HIS
1	A	323	ASN
1	B	62	HIS
1	B	94	HIS
1	B	129	ASN
1	B	151	ASN
1	B	155	ASN
1	B	172	GLN

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Mol	Chain	Res	Type
1	B	177	ASN
1	B	202	ASN
1	B	323	ASN
1	C	129	ASN
1	C	151	ASN
1	C	155	ASN
1	C	161	GLN
1	C	172	GLN
1	C	177	ASN
1	C	202	ASN
1	C	205	HIS
1	C	286	HIS
1	C	323	ASN
1	D	94	HIS
1	D	129	ASN
1	D	155	ASN
1	D	172	GLN
1	D	177	ASN
1	D	202	ASN
1	D	205	HIS
1	D	323	ASN

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.