



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID : 1GG3
Title : CRYSTAL STRUCTURE OF THE PROTEIN 4.1R MEMBRANE BINDING DOMAIN
Authors : Han, B.G.
Deposited on : 2000-07-11
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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

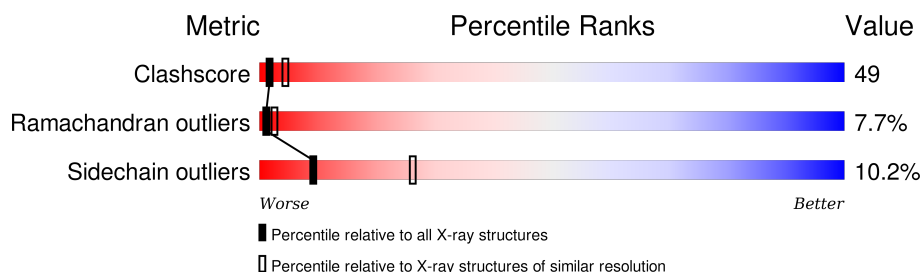
1 Overall quality at a glance

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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 $\leq 5\%$. 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	279	 41% 44% 14%
1	B	279	 43% 48% 9% •
1	C	279	 33% 53% 13% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6837 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 ERYTHROID MEMBRANE PROTEIN 4.1R.

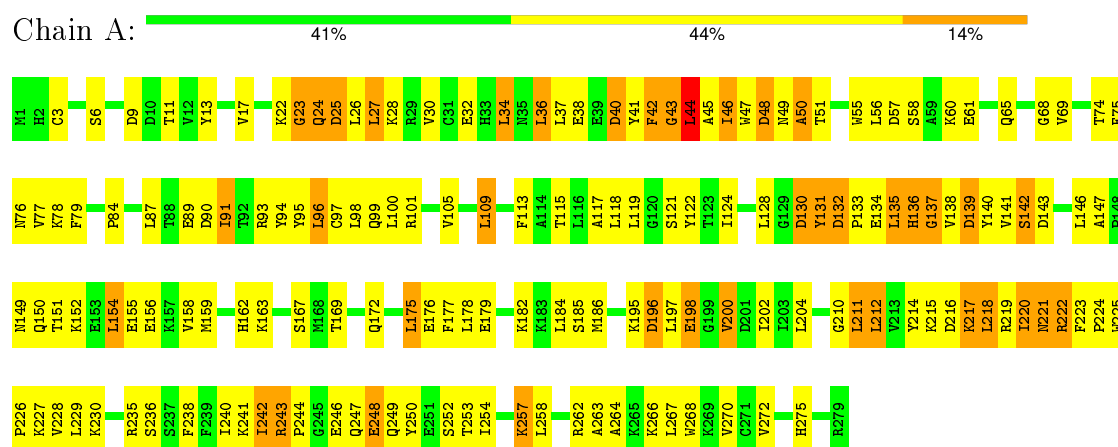
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2279	1472	380	416	11			
1	B	279	Total	C	N	O	S	0	0	0
			2279	1472	380	416	11			
1	C	279	Total	C	N	O	S	0	0	0
			2279	1472	380	416	11			

3 Residue-property plots

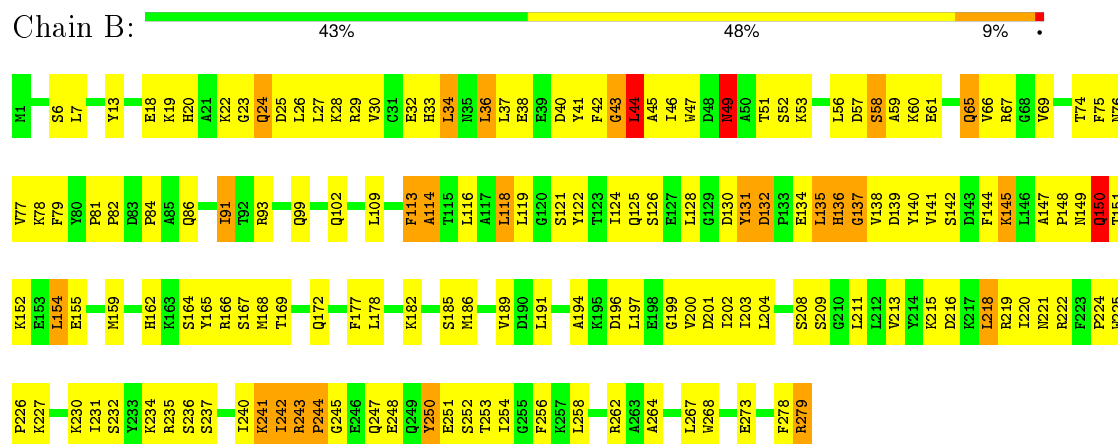
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

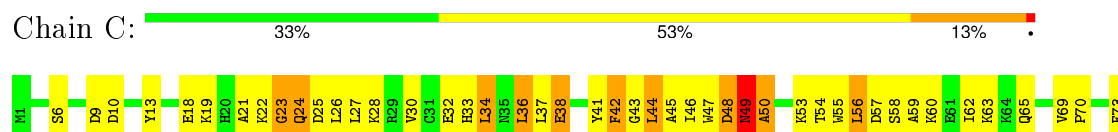
• Molecule 1: ERYTHROID MEMBRANE PROTEIN 4.1R



• Molecule 1: ERYTHROID MEMBRANE PROTEIN 4.1R



• Molecule 1: ERYTHROID MEMBRANE PROTEIN 4.1R



[illegible]

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.90 Å 106.50 Å 93.50 Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.226 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6837	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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	0.46	0/2335	0.71	1/3154 (0.0%)
1	B	0.47	0/2335	0.73	2/3154 (0.1%)
1	C	0.49	0/2335	0.76	1/3154 (0.0%)
All	All	0.48	0/7005	0.73	4/9462 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	LEU	N-CA-C	-5.77	95.43	111.00
1	B	135	LEU	N-CA-C	-5.59	95.92	111.00
1	A	135	LEU	N-CA-C	-5.30	96.69	111.00
1	B	134	GLU	N-CA-C	-5.30	96.69	111.00

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	2279	0	2287	235	0
1	B	2279	0	2287	196	1
1	C	2279	0	2287	251	1
All	All	6837	0	6861	667	2

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 49.

All (667) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLY:HA2	1:B:79:PHE:H	1.06	1.15
1:A:43:GLY:HA2	1:A:79:PHE:H	1.02	1.12
1:A:229:LEU:HG	1:A:242:ILE:HG12	1.31	1.10
1:C:196:ASP:HB3	1:C:200:VAL:HB	1.32	1.07
1:A:24:GLN:HB2	1:A:28:LYS:HB2	1.35	1.06
1:B:91:ILE:HD13	1:B:91:ILE:H	1.17	1.05
1:A:43:GLY:HA3	1:A:77:VAL:HG13	1.36	1.03
1:C:215:LYS:HB2	1:C:220:ILE:HD11	1.40	1.01
1:C:229:LEU:H	1:C:242:ILE:HD13	1.21	1.01
1:C:229:LEU:HB2	1:C:242:ILE:HG12	1.43	0.99
1:C:19:LYS:HE2	1:C:63:LYS:HE2	1.44	0.96
1:C:131:TYR:O	1:C:135:LEU:HD22	1.66	0.95
1:C:6:SER:HB3	1:C:74:THR:HG22	1.45	0.95
1:A:43:GLY:HA2	1:A:79:PHE:N	1.81	0.95
1:B:43:GLY:HA2	1:B:79:PHE:N	1.83	0.93
1:B:244:PRO:HB3	1:B:247:GLN:HE21	1.32	0.92
1:B:149:ASN:O	1:B:150:GLN:HB2	1.66	0.91
1:A:258:LEU:HD22	1:A:264:ALA:HA	1.52	0.91
1:C:215:LYS:CB	1:C:220:ILE:HD11	2.02	0.90
1:A:57:ASP:H	1:A:65:GLN:HE22	0.96	0.90
1:B:222:ARG:O	1:B:224:PRO:HD3	1.72	0.90
1:C:43:GLY:HA2	1:C:79:PHE:H	1.36	0.89
1:C:229:LEU:HD23	1:C:242:ILE:HG21	1.53	0.88
1:B:24:GLN:HB2	1:B:28:LYS:HZ2	1.36	0.88
1:B:43:GLY:CA	1:B:79:PHE:H	1.87	0.87
1:B:43:GLY:CA	1:B:78:LYS:H	1.86	0.87
1:C:227:LYS:HG3	1:C:243:ARG:HB2	1.57	0.87
1:C:212:LEU:HD22	1:C:222:ARG:HG3	1.57	0.87
1:A:43:GLY:C	1:A:78:LYS:H	1.78	0.86
1:A:28:LYS:HB3	1:A:28:LYS:NZ	1.90	0.86
1:C:24:GLN:HB2	1:C:28:LYS:HB2	1.56	0.86
1:C:242:ILE:HG22	1:C:243:ARG:HG2	1.58	0.85
1:B:77:VAL:H	1:B:99:GLN:HE21	1.22	0.85
1:B:6:SER:HB3	1:B:74:THR:HG22	1.59	0.85
1:B:222:ARG:NH1	1:B:224:PRO:HG3	1.91	0.85
1:C:24:GLN:H	1:C:56:LEU:HD13	1.41	0.85
1:A:222:ARG:O	1:A:224:PRO:HD3	1.76	0.85
1:C:47:TRP:CZ3	1:C:49:ASN:HA	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASP:HB3	1:A:200:VAL:HG23	1.57	0.84
1:B:169:THR:OG1	1:B:172:GLN:HG3	1.75	0.84
1:C:13:TYR:CE1	1:C:34:LEU:HG	2.13	0.84
1:A:244:PRO:HG2	1:A:250:TYR:CB	2.08	0.84
1:A:210:GLY:HA2	1:A:225:TRP:CE2	2.13	0.83
1:A:57:ASP:H	1:A:65:GLN:NE2	1.75	0.83
1:C:229:LEU:H	1:C:242:ILE:CD1	1.93	0.82
1:B:42:PHE:O	1:B:44:LEU:N	2.13	0.82
1:C:24:GLN:HG2	1:C:58:SER:HA	1.61	0.81
1:A:131:TYR:O	1:A:135:LEU:HD22	1.80	0.81
1:B:28:LYS:NZ	1:B:28:LYS:HB3	1.94	0.81
1:A:28:LYS:HD2	1:A:45:ALA:HA	1.62	0.81
1:C:169:THR:H	1:C:172:GLN:NE2	1.77	0.81
1:B:222:ARG:HH12	1:B:224:PRO:HG3	1.45	0.81
1:C:44:LEU:H	1:C:77:VAL:HA	1.44	0.80
1:B:46:ILE:HG22	1:B:75:PHE:HA	1.63	0.80
1:C:219:ARG:HH12	1:C:222:ARG:HB2	1.47	0.80
1:C:212:LEU:HD13	1:C:219:ARG:HD2	1.61	0.80
1:C:217:LYS:HB2	1:C:218:LEU:HD22	1.64	0.80
1:B:43:GLY:C	1:B:78:LYS:H	1.85	0.80
1:A:241:LYS:HG2	1:A:253:THR:HG23	1.64	0.79
1:A:244:PRO:HB2	1:A:247:GLN:HE21	1.44	0.79
1:C:57:ASP:H	1:C:65:GLN:HE22	1.30	0.79
1:B:258:LEU:CD1	1:B:264:ALA:HA	2.13	0.79
1:B:222:ARG:HG2	1:B:222:ARG:HH11	1.47	0.78
1:C:241:LYS:C	1:C:242:ILE:HD12	2.04	0.78
1:A:254:ILE:H	1:A:254:ILE:HD12	1.49	0.77
1:B:24:GLN:HB2	1:B:28:LYS:HB2	1.65	0.77
1:A:244:PRO:HG2	1:A:250:TYR:HB3	1.67	0.77
1:C:125:GLN:HG3	1:C:168:MET:CE	2.15	0.77
1:C:28:LYS:HA	1:C:46:ILE:HD11	1.68	0.76
1:B:244:PRO:HB3	1:B:247:GLN:NE2	1.99	0.76
1:B:243:ARG:HB3	1:B:244:PRO:CD	2.15	0.76
1:A:169:THR:H	1:A:172:GLN:NE2	1.84	0.75
1:B:43:GLY:CA	1:B:78:LYS:N	2.49	0.75
1:C:254:ILE:N	1:C:254:ILE:HD12	2.00	0.74
1:A:185:SER:O	1:A:186:MET:HB2	1.86	0.74
1:C:132:ASP:H	1:C:166:ARG:NH2	1.86	0.73
1:B:49:ASN:H	1:B:49:ASN:ND2	1.84	0.73
1:B:28:LYS:NZ	1:B:28:LYS:CB	2.50	0.73
1:B:43:GLY:HA3	1:B:77:VAL:HG13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PHE:O	1:B:43:GLY:C	2.27	0.72
1:C:23:GLY:O	1:C:25:ASP:N	2.22	0.72
1:A:147:ALA:O	1:A:150:GLN:HG2	1.89	0.72
1:A:43:GLY:HA3	1:A:77:VAL:CG1	2.17	0.72
1:A:32:GLU:OE2	1:A:32:GLU:HA	1.90	0.72
1:C:229:LEU:N	1:C:242:ILE:HD13	2.01	0.72
1:C:134:GLU:HG3	1:C:135:LEU:HD13	1.72	0.72
1:B:28:LYS:HZ3	1:B:28:LYS:HB3	1.53	0.72
1:B:149:ASN:ND2	1:B:150:GLN:H	1.86	0.71
1:C:197:LEU:O	1:C:198:GLU:HB2	1.88	0.71
1:B:258:LEU:HD13	1:B:264:ALA:HA	1.71	0.71
1:A:36:LEU:HD13	1:B:262:ARG:HH21	1.56	0.71
1:B:47:TRP:CZ3	1:B:49:ASN:HA	2.26	0.71
1:C:185:SER:O	1:C:186:MET:HB2	1.88	0.71
1:B:230:LYS:HB3	1:B:241:LYS:HG2	1.72	0.70
1:C:44:LEU:HD12	1:C:75:PHE:CE1	2.27	0.70
1:B:119:LEU:HB3	1:B:177:PHE:CE2	2.26	0.70
1:C:125:GLN:HE21	1:C:162:HIS:HE1	1.38	0.70
1:C:91:ILE:N	1:C:91:ILE:HD12	2.07	0.70
1:B:28:LYS:O	1:B:32:GLU:HG2	1.92	0.70
1:B:243:ARG:HB3	1:B:244:PRO:HD2	1.73	0.70
1:B:131:TYR:O	1:B:135:LEU:HD22	1.91	0.69
1:A:13:TYR:CE1	1:A:34:LEU:HG	2.27	0.69
1:A:42:PHE:O	1:A:43:GLY:C	2.30	0.69
1:C:47:TRP:NE1	1:C:76:ASN:OD1	2.25	0.69
1:C:91:ILE:HD12	1:C:91:ILE:H	1.56	0.69
1:C:23:GLY:HA2	1:C:62:ILE:CG1	2.22	0.69
1:C:196:ASP:HB3	1:C:200:VAL:CB	2.17	0.69
1:A:149:ASN:HD22	1:A:151:THR:HG23	1.57	0.69
1:A:43:GLY:CA	1:A:78:LYS:H	2.05	0.69
1:A:244:PRO:HB2	1:A:247:GLN:NE2	2.07	0.69
1:C:226:PRO:O	1:C:227:LYS:HB3	1.91	0.69
1:B:244:PRO:HG2	1:B:248:GLU:HA	1.72	0.69
1:B:38:GLU:OE1	1:B:38:GLU:HA	1.92	0.69
1:B:43:GLY:O	1:B:44:LEU:C	2.30	0.69
1:B:149:ASN:CG	1:B:150:GLN:H	1.96	0.68
1:A:243:ARG:NH2	1:A:244:PRO:HD2	2.07	0.68
1:C:22:LYS:HD3	1:C:59:ALA:HA	1.74	0.68
1:C:24:GLN:O	1:C:25:ASP:C	2.32	0.68
1:C:43:GLY:CA	1:C:79:PHE:H	2.06	0.68
1:C:258:LEU:HD11	1:C:267:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:HG2	1:A:250:TYR:HB2	1.76	0.68
1:C:23:GLY:HA2	1:C:62:ILE:HG13	1.76	0.68
1:B:204:LEU:HD12	1:B:267:LEU:HD21	1.74	0.68
1:A:134:GLU:HA	1:A:136:HIS:CE1	2.30	0.67
1:A:215:LYS:CB	1:A:220:ILE:HD11	2.24	0.67
1:C:141:VAL:HG12	1:C:141:VAL:O	1.94	0.67
1:A:77:VAL:HB	1:A:99:GLN:HG2	1.76	0.67
1:C:43:GLY:CA	1:C:78:LYS:H	2.07	0.67
1:A:57:ASP:N	1:A:65:GLN:HE22	1.82	0.67
1:A:211:LEU:HD12	1:A:240:ILE:HG21	1.77	0.67
1:C:87:LEU:HD13	1:C:92:THR:HG22	1.77	0.67
1:A:109:LEU:HD22	1:A:184:LEU:HD13	1.76	0.66
1:C:43:GLY:O	1:C:44:LEU:HB2	1.95	0.66
1:C:236:SER:HB2	1:C:258:LEU:O	1.95	0.66
1:A:47:TRP:NE1	1:A:76:ASN:OD1	2.28	0.66
1:A:24:GLN:HB2	1:A:28:LYS:CB	2.20	0.66
1:C:125:GLN:HE21	1:C:162:HIS:CE1	2.13	0.66
1:B:13:TYR:CE1	1:B:34:LEU:HG	2.30	0.66
1:A:43:GLY:CA	1:A:79:PHE:H	1.95	0.66
1:C:45:ALA:HB3	1:C:55:TRP:CZ3	2.31	0.66
1:C:237:SER:HB3	1:C:239:PHE:CZ	2.31	0.65
1:A:47:TRP:HZ3	1:A:49:ASN:HA	1.62	0.65
1:B:24:GLN:O	1:B:28:LYS:N	2.30	0.65
1:A:97:CYS:O	1:A:101:ARG:HG3	1.97	0.65
1:B:118:LEU:HD22	1:B:122:TYR:CE1	2.31	0.65
1:B:43:GLY:HA2	1:B:78:LYS:N	2.10	0.65
1:A:242:ILE:HG13	1:A:243:ARG:N	2.11	0.65
1:C:43:GLY:HA2	1:C:78:LYS:H	1.62	0.65
1:A:28:LYS:HB3	1:A:28:LYS:HZ3	1.61	0.64
1:C:243:ARG:HH22	1:C:248:GLU:HA	1.62	0.64
1:B:24:GLN:H	1:B:56:LEU:CD1	2.10	0.64
1:C:24:GLN:O	1:C:28:LYS:N	2.28	0.64
1:A:268:TRP:O	1:A:272:VAL:HG23	1.97	0.64
1:A:28:LYS:HB3	1:A:28:LYS:HZ2	1.61	0.64
1:B:258:LEU:HD11	1:B:267:LEU:HD23	1.80	0.64
1:C:132:ASP:H	1:C:166:ARG:HH22	1.46	0.64
1:C:19:LYS:HE2	1:C:63:LYS:CE	2.24	0.64
1:A:215:LYS:HE3	1:A:220:ILE:CD1	2.28	0.64
1:C:212:LEU:CD2	1:C:222:ARG:HG3	2.27	0.63
1:A:140:TYR:OH	1:A:162:HIS:HD2	1.81	0.63
1:B:77:VAL:H	1:B:99:GLN:NE2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HA	1:A:76:ASN:O	1.98	0.63
1:A:196:ASP:HB3	1:A:200:VAL:CG2	2.25	0.63
1:B:125:GLN:HG3	1:B:168:MET:CE	2.29	0.63
1:B:254:ILE:N	1:B:254:ILE:HD12	2.14	0.63
1:A:258:LEU:HD22	1:A:264:ALA:CA	2.26	0.63
1:C:122:TYR:CE1	1:C:176:GLU:HB3	2.33	0.63
1:A:87:LEU:O	1:A:93:ARG:NH2	2.32	0.63
1:C:227:LYS:NZ	1:C:227:LYS:HB2	2.14	0.63
1:B:28:LYS:HZ2	1:B:28:LYS:CB	2.10	0.62
1:B:222:ARG:NH1	1:B:222:ARG:HG2	2.11	0.62
1:A:247:GLN:O	1:A:247:GLN:HG2	2.00	0.62
1:B:23:GLY:O	1:B:25:ASP:N	2.32	0.62
1:C:226:PRO:O	1:C:227:LYS:CB	2.47	0.62
1:C:189:VAL:HG22	1:C:207:CYS:HB3	1.81	0.62
1:B:145:LYS:HD3	1:B:145:LYS:N	2.14	0.62
1:C:131:TYR:CE1	1:C:163:LYS:HE2	2.35	0.62
1:A:25:ASP:HB2	1:A:58:SER:O	2.00	0.62
1:C:222:ARG:O	1:C:224:PRO:HD3	1.99	0.62
1:C:46:ILE:HG22	1:C:73:PHE:HB3	1.81	0.62
1:A:225:TRP:HB2	1:A:226:PRO:HD3	1.81	0.61
1:B:230:LYS:HB3	1:B:241:LYS:CG	2.30	0.61
1:A:218:LEU:C	1:A:220:ILE:H	2.03	0.61
1:A:204:LEU:HD12	1:A:267:LEU:HD21	1.82	0.61
1:B:26:LEU:O	1:B:30:VAL:HG23	2.00	0.61
1:B:28:LYS:HD3	1:B:45:ALA:HA	1.83	0.61
1:B:125:GLN:HG3	1:B:168:MET:HE2	1.81	0.61
1:C:37:LEU:HD21	1:C:95:TYR:HD1	1.65	0.61
1:C:47:TRP:NE1	1:C:74:THR:OG1	2.33	0.61
1:B:236:SER:HB2	1:B:258:LEU:O	2.01	0.61
1:C:141:VAL:HG21	1:C:159:MET:HG2	1.83	0.61
1:B:28:LYS:CD	1:B:45:ALA:HA	2.30	0.60
1:A:242:ILE:HG13	1:A:243:ARG:H	1.66	0.60
1:A:185:SER:O	1:A:186:MET:CB	2.49	0.60
1:A:6:SER:HB3	1:A:74:THR:HG22	1.82	0.60
1:A:219:ARG:HB3	1:A:219:ARG:NH1	2.15	0.60
1:A:22:LYS:O	1:A:23:GLY:O	2.19	0.60
1:A:229:LEU:CG	1:A:242:ILE:HG12	2.19	0.60
1:C:121:SER:HB2	1:C:165:TYR:HE1	1.66	0.60
1:C:139:ASP:O	1:C:141:VAL:N	2.35	0.60
1:C:131:TYR:CZ	1:C:163:LYS:HE2	2.36	0.60
1:C:225:TRP:HB2	1:C:226:PRO:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:NE	1:C:36:LEU:HD13	2.17	0.60
1:B:142:SER:HA	1:B:155:GLU:OE2	2.01	0.60
1:A:28:LYS:CB	1:A:28:LYS:NZ	2.65	0.60
1:B:227:LYS:NZ	1:B:245:GLY:HA2	2.17	0.60
1:A:124:ILE:HG23	1:A:128:LEU:HD12	1.82	0.60
1:A:154:LEU:O	1:A:154:LEU:HD22	2.01	0.60
1:C:152:LYS:O	1:C:156:GLU:HG2	2.02	0.60
1:B:77:VAL:HB	1:B:99:GLN:HG2	1.84	0.60
1:A:258:LEU:N	1:A:258:LEU:HD12	2.17	0.60
1:C:84:PRO:HB2	1:C:178:LEU:HD13	1.84	0.60
1:A:230:LYS:HD3	1:A:241:LYS:HD2	1.83	0.60
1:C:116:LEU:HD21	1:C:147:ALA:CB	2.32	0.60
1:B:24:GLN:HG3	1:B:58:SER:OG	2.02	0.60
1:C:13:TYR:HE1	1:C:34:LEU:HG	1.64	0.59
1:A:142:SER:HA	1:A:155:GLU:OE2	2.02	0.59
1:B:91:ILE:HD13	1:B:91:ILE:N	2.02	0.59
1:A:134:GLU:C	1:A:136:HIS:H	2.05	0.59
1:B:57:ASP:H	1:B:65:GLN:HE22	1.48	0.59
1:A:152:LYS:O	1:A:156:GLU:HG2	2.02	0.59
1:A:24:GLN:HG2	1:A:58:SER:HA	1.85	0.59
1:C:175:LEU:HD13	1:C:175:LEU:O	2.03	0.59
1:C:41:TYR:O	1:C:43:GLY:O	2.21	0.59
1:A:36:LEU:HD13	1:A:36:LEU:O	2.02	0.58
1:C:185:SER:O	1:C:186:MET:CB	2.51	0.58
1:C:241:LYS:CG	1:C:242:ILE:HD12	2.33	0.58
1:A:254:ILE:HD12	1:A:254:ILE:N	2.14	0.58
1:B:140:TYR:OH	1:B:162:HIS:HD2	1.86	0.58
1:A:241:LYS:O	1:A:242:ILE:HB	2.03	0.58
1:C:125:GLN:NE2	1:C:129:GLY:O	2.36	0.58
1:A:149:ASN:O	1:A:150:GLN:HB2	2.02	0.58
1:A:55:TRP:CE2	1:A:78:LYS:HG3	2.39	0.58
1:C:42:PHE:O	1:C:44:LEU:HD22	2.04	0.58
1:B:130:ASP:OD1	1:B:167:SER:N	2.29	0.58
1:A:32:GLU:HG3	1:A:40:ASP:OD2	2.03	0.58
1:A:36:LEU:HD11	1:B:262:ARG:HE	1.69	0.58
1:C:217:LYS:CB	1:C:218:LEU:HD22	2.34	0.58
1:C:22:LYS:O	1:C:23:GLY:O	2.21	0.57
1:C:21:ALA:HB1	1:C:26:LEU:HD12	1.85	0.57
1:A:93:ARG:HD3	1:A:175:LEU:CD2	2.34	0.57
1:B:49:ASN:HD22	1:B:49:ASN:H	1.51	0.57
1:A:32:GLU:CA	1:A:32:GLU:OE2	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LYS:HG3	1:C:243:ARG:CB	2.33	0.57
1:C:44:LEU:HG	1:C:75:PHE:HZ	1.70	0.57
1:A:236:SER:HB2	1:A:258:LEU:O	2.04	0.57
1:A:212:LEU:HD22	1:A:222:ARG:HG3	1.86	0.57
1:A:215:LYS:HE3	1:A:220:ILE:HD11	1.87	0.57
1:A:36:LEU:CD1	1:B:262:ARG:HE	2.18	0.57
1:B:36:LEU:O	1:B:36:LEU:HD13	2.04	0.57
1:B:136:HIS:O	1:B:137:GLY:O	2.22	0.57
1:A:248:GLU:O	1:A:250:TYR:N	2.35	0.57
1:C:231:ILE:HG23	1:C:240:ILE:HG22	1.86	0.57
1:A:28:LYS:CD	1:A:45:ALA:HA	2.31	0.57
1:A:49:ASN:O	1:A:50:ALA:CB	2.53	0.57
1:A:215:LYS:HB2	1:A:220:ILE:HD11	1.85	0.57
1:C:115:THR:C	1:C:117:ALA:H	2.06	0.57
1:C:140:TYR:OH	1:C:162:HIS:HD2	1.86	0.56
1:B:253:THR:C	1:B:254:ILE:HD12	2.25	0.56
1:B:24:GLN:O	1:B:25:ASP:C	2.44	0.56
1:A:262:ARG:NE	1:C:36:LEU:CD1	2.68	0.56
1:B:19:LYS:HE2	1:B:20:HIS:NE2	2.20	0.56
1:B:113:PHE:O	1:B:114:ALA:HB2	2.04	0.56
1:B:22:LYS:H	1:B:26:LEU:HD12	1.71	0.56
1:A:229:LEU:HB2	1:A:242:ILE:HB	1.88	0.56
1:A:43:GLY:CA	1:A:78:LYS:N	2.69	0.56
1:B:24:GLN:HG2	1:B:58:SER:HA	1.88	0.56
1:B:47:TRP:HZ3	1:B:49:ASN:HA	1.71	0.56
1:B:196:ASP:OD2	1:B:200:VAL:HB	2.05	0.56
1:C:47:TRP:CD1	1:C:76:ASN:OD1	2.59	0.56
1:C:47:TRP:HE3	1:C:48:ASP:O	1.89	0.55
1:B:250:TYR:HE1	1:B:252:SER:HB3	1.71	0.55
1:C:169:THR:N	1:C:172:GLN:NE2	2.53	0.55
1:A:101:ARG:O	1:A:105:VAL:HG23	2.06	0.55
1:C:214:TYR:CE2	1:C:219:ARG:HG2	2.41	0.55
1:A:262:ARG:NH2	1:C:36:LEU:O	2.38	0.55
1:C:111:CYS:SG	1:C:116:LEU:HB2	2.47	0.55
1:B:24:GLN:HB2	1:B:28:LYS:CB	2.33	0.55
1:B:219:ARG:NH2	1:B:222:ARG:HD2	2.22	0.55
1:C:23:GLY:O	1:C:24:GLN:C	2.45	0.55
1:C:131:TYR:O	1:C:135:LEU:CD2	2.49	0.55
1:A:219:ARG:O	1:A:221:ASN:N	2.39	0.55
1:A:42:PHE:O	1:A:44:LEU:N	2.39	0.55
1:A:215:LYS:HB3	1:A:220:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:HE21	1:B:162:HIS:CE1	2.24	0.55
1:C:57:ASP:H	1:C:65:GLN:NE2	2.01	0.55
1:C:141:VAL:CG2	1:C:159:MET:HG2	2.37	0.55
1:C:53:LYS:O	1:C:266:LYS:HE3	2.07	0.55
1:B:7:LEU:HD11	1:B:13:TYR:HB2	1.88	0.55
1:C:266:LYS:O	1:C:270:VAL:HG23	2.06	0.54
1:A:196:ASP:O	1:A:198:GLU:N	2.40	0.54
1:B:46:ILE:HG22	1:B:75:PHE:CA	2.35	0.54
1:A:229:LEU:HD12	1:A:242:ILE:HD13	1.89	0.54
1:B:91:ILE:H	1:B:91:ILE:CD1	1.99	0.54
1:B:227:LYS:HE2	1:B:242:ILE:HD11	1.88	0.54
1:C:254:ILE:N	1:C:254:ILE:CD1	2.71	0.54
1:B:186:MET:HE2	1:B:186:MET:HA	1.89	0.54
1:A:266:LYS:O	1:A:270:VAL:HG23	2.07	0.54
1:C:19:LYS:CE	1:C:63:LYS:HE2	2.29	0.54
1:C:47:TRP:CD1	1:C:74:THR:OG1	2.60	0.54
1:A:195:LYS:HG3	1:A:200:VAL:O	2.08	0.54
1:C:257:LYS:HG3	1:C:257:LYS:O	2.07	0.54
1:A:43:GLY:O	1:A:44:LEU:C	2.45	0.54
1:C:241:LYS:HG3	1:C:242:ILE:HD12	1.90	0.54
1:B:118:LEU:O	1:B:121:SER:OG	2.21	0.54
1:C:36:LEU:HD13	1:C:36:LEU:O	2.08	0.54
1:B:244:PRO:HG3	1:B:250:TYR:O	2.08	0.54
1:B:132:ASP:OD1	1:B:132:ASP:C	2.45	0.54
1:B:225:TRP:HB2	1:B:226:PRO:HD3	1.90	0.54
1:A:36:LEU:HD11	1:B:262:ARG:NE	2.24	0.53
1:C:91:ILE:CD1	1:C:91:ILE:H	2.16	0.53
1:B:235:ARG:NE	1:B:235:ARG:HA	2.22	0.53
1:B:43:GLY:HA3	1:B:77:VAL:CG1	2.37	0.53
1:C:87:LEU:HD13	1:C:92:THR:CG2	2.38	0.53
1:B:49:ASN:N	1:B:49:ASN:ND2	2.55	0.53
1:B:24:GLN:H	1:B:56:LEU:HD12	1.73	0.53
1:A:43:GLY:HA2	1:A:78:LYS:N	2.24	0.53
1:C:228:VAL:C	1:C:229:LEU:HD22	2.29	0.53
1:C:89:GLU:HB3	1:C:91:ILE:CD1	2.38	0.53
1:C:258:LEU:HD13	1:C:264:ALA:HA	1.91	0.53
1:B:141:VAL:HB	1:B:159:MET:HE2	1.91	0.53
1:C:241:LYS:HB2	1:C:252:SER:O	2.09	0.53
1:C:23:GLY:HA2	1:C:62:ILE:HG12	1.90	0.53
1:A:24:GLN:CB	1:A:28:LYS:HB2	2.24	0.53
1:A:47:TRP:HE1	1:A:76:ASN:CG	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLU:CG	1:C:135:LEU:HD13	2.38	0.53
1:C:28:LYS:CA	1:C:46:ILE:HD11	2.37	0.53
1:B:165:TYR:CG	1:B:168:MET:HE1	2.44	0.53
1:A:23:GLY:O	1:A:25:ASP:N	2.42	0.53
1:C:116:LEU:HD21	1:C:147:ALA:HB2	1.90	0.53
1:A:202:ILE:C	1:A:202:ILE:HD12	2.29	0.53
1:B:215:LYS:HB3	1:B:220:ILE:HD11	1.90	0.53
1:B:258:LEU:HD12	1:B:264:ALA:HA	1.90	0.53
1:A:119:LEU:HB3	1:A:177:PHE:CE2	2.44	0.53
1:A:50:ALA:O	1:A:51:THR:HB	2.08	0.53
1:A:211:LEU:HD13	1:A:240:ILE:HD13	1.91	0.53
1:A:154:LEU:O	1:A:158:VAL:HG23	2.08	0.52
1:A:91:ILE:O	1:A:94:TYR:HB3	2.08	0.52
1:A:47:TRP:CZ3	1:A:49:ASN:HA	2.44	0.52
1:B:51:THR:HG22	1:B:52:SER:N	2.25	0.52
1:C:205:GLY:O	1:C:211:LEU:HD23	2.10	0.52
1:A:134:GLU:C	1:A:136:HIS:N	2.63	0.52
1:A:225:TRP:CE3	1:A:275:HIS:HB2	2.44	0.52
1:C:175:LEU:O	1:C:179:GLU:HG2	2.10	0.52
1:A:229:LEU:HG	1:A:242:ILE:CG1	2.22	0.52
1:C:23:GLY:N	1:C:60:LYS:O	2.29	0.52
1:A:84:PRO:HD2	1:A:182:LYS:HG3	1.91	0.52
1:A:241:LYS:O	1:A:242:ILE:CB	2.58	0.52
1:C:197:LEU:O	1:C:198:GLU:CB	2.57	0.52
1:B:235:ARG:HG2	1:B:235:ARG:NH1	2.24	0.52
1:A:9:ASP:OD2	1:A:11:THR:HB	2.10	0.52
1:C:214:TYR:CZ	1:C:219:ARG:HG2	2.45	0.51
1:C:254:ILE:HG22	1:C:255:GLY:N	2.25	0.51
1:B:121:SER:HB2	1:B:165:TYR:CE1	2.45	0.51
1:B:125:GLN:HE22	1:B:130:ASP:HA	1.74	0.51
1:B:235:ARG:HG2	1:B:235:ARG:HH11	1.75	0.51
1:B:215:LYS:O	1:B:216:ASP:HB2	2.09	0.51
1:C:235:ARG:HA	1:C:235:ARG:NE	2.25	0.51
1:C:215:LYS:HB3	1:C:220:ILE:HD11	1.89	0.51
1:C:241:LYS:HG3	1:C:242:ILE:CD1	2.40	0.51
1:A:254:ILE:CD1	1:A:254:ILE:H	2.23	0.51
1:C:268:TRP:O	1:C:272:VAL:HG23	2.10	0.51
1:B:218:LEU:N	1:B:218:LEU:HD22	2.26	0.51
1:A:243:ARG:HA	1:A:243:ARG:NE	2.24	0.51
1:C:89:GLU:HB3	1:C:91:ILE:HD11	1.91	0.51
1:A:113:PHE:CZ	1:A:154:LEU:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:HA	1:A:242:ILE:CG2	2.41	0.51
1:A:242:ILE:HG13	1:A:243:ARG:HG2	1.92	0.51
1:C:227:LYS:HB2	1:C:227:LYS:HZ3	1.75	0.51
1:A:146:LEU:N	1:A:150:GLN:OE1	2.41	0.51
1:A:229:LEU:N	1:A:242:ILE:HG21	2.26	0.51
1:C:47:TRP:CE3	1:C:48:ASP:O	2.63	0.51
1:A:225:TRP:C	1:A:227:LYS:H	2.14	0.51
1:A:139:ASP:HA	1:A:159:MET:CE	2.41	0.51
1:A:47:TRP:HE3	1:A:48:ASP:C	2.14	0.51
1:B:186:MET:CE	1:B:186:MET:HA	2.40	0.51
1:C:210:GLY:HA3	1:C:223:PHE:O	2.11	0.51
1:C:43:GLY:HA3	1:C:77:VAL:HG13	1.92	0.51
1:C:145:LYS:HD3	1:C:145:LYS:H	1.76	0.51
1:B:78:LYS:HE2	1:B:273:GLU:OE1	2.11	0.50
1:C:213:VAL:C	1:C:214:TYR:HD2	2.15	0.50
1:A:124:ILE:CG2	1:A:128:LEU:HD12	2.40	0.50
1:C:113:PHE:CZ	1:C:154:LEU:HA	2.46	0.50
1:B:137:GLY:C	1:B:139:ASP:H	2.14	0.50
1:A:94:TYR:CE2	1:B:67:ARG:HD2	2.46	0.50
1:A:24:GLN:O	1:A:28:LYS:N	2.43	0.50
1:B:185:SER:O	1:B:186:MET:HB2	2.10	0.50
1:B:234:LYS:O	1:B:237:SER:HB2	2.12	0.50
1:C:248:GLU:O	1:C:249:GLN:HB2	2.12	0.50
1:A:263:ALA:O	1:A:266:LYS:HB3	2.12	0.50
1:C:44:LEU:HA	1:C:76:ASN:O	2.12	0.50
1:B:240:ILE:C	1:B:241:LYS:HD3	2.33	0.50
1:A:24:GLN:O	1:A:26:LEU:N	2.45	0.49
1:A:43:GLY:HA2	1:A:78:LYS:H	1.77	0.49
1:B:145:LYS:HD3	1:B:145:LYS:H	1.77	0.49
1:B:23:GLY:O	1:B:24:GLN:C	2.50	0.49
1:A:247:GLN:HG3	1:A:250:TYR:CG	2.48	0.49
1:A:178:LEU:O	1:A:182:LYS:HB2	2.12	0.49
1:C:198:GLU:HB3	1:C:200:VAL:CG2	2.42	0.49
1:A:215:LYS:HB2	1:A:220:ILE:CD1	2.42	0.49
1:C:138:VAL:HG13	1:C:159:MET:HE3	1.93	0.49
1:C:130:ASP:CG	1:C:167:SER:H	2.16	0.49
1:A:149:ASN:ND2	1:A:150:GLN:H	2.11	0.49
1:C:69:VAL:HG12	1:C:70:PRO:O	2.13	0.49
1:C:243:ARG:NH2	1:C:248:GLU:HA	2.26	0.49
1:C:24:GLN:HG2	1:C:58:SER:CA	2.39	0.49
1:A:186:MET:CE	1:A:186:MET:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:CG	1:A:150:GLN:H	2.16	0.49
1:C:144:PHE:O	1:C:146:LEU:HG	2.11	0.49
1:C:225:TRP:CE3	1:C:225:TRP:HA	2.47	0.48
1:B:141:VAL:HB	1:B:159:MET:CE	2.43	0.48
1:C:215:LYS:HB2	1:C:220:ILE:CD1	2.28	0.48
1:C:49:ASN:O	1:C:50:ALA:HB3	2.13	0.48
1:B:219:ARG:CZ	1:B:222:ARG:HD2	2.43	0.48
1:C:73:PHE:N	1:C:73:PHE:CD1	2.81	0.48
1:C:90:ASP:OD1	1:C:93:ARG:NH1	2.46	0.48
1:C:242:ILE:CG2	1:C:243:ARG:HG2	2.36	0.48
1:C:24:GLN:CG	1:C:58:SER:HA	2.38	0.48
1:C:216:ASP:O	1:C:217:LYS:HG2	2.13	0.48
1:A:262:ARG:CZ	1:C:36:LEU:HD13	2.43	0.48
1:B:231:ILE:HG22	1:B:268:TRP:HD1	1.79	0.48
1:B:44:LEU:H	1:B:44:LEU:HD13	1.79	0.48
1:B:149:ASN:CG	1:B:150:GLN:N	2.66	0.48
1:A:146:LEU:HB2	1:A:150:GLN:OE1	2.14	0.48
1:B:61:GLU:O	1:B:65:GLN:HG3	2.13	0.48
1:B:84:PRO:HB2	1:B:178:LEU:HD13	1.95	0.48
1:C:242:ILE:HG22	1:C:243:ARG:N	2.29	0.48
1:C:53:LYS:HZ2	1:C:55:TRP:HZ2	1.62	0.48
1:B:23:GLY:N	1:B:60:LYS:O	2.44	0.47
1:A:28:LYS:CB	1:A:28:LYS:HZ2	2.23	0.47
1:A:242:ILE:CG1	1:A:243:ARG:H	2.27	0.47
1:B:241:LYS:N	1:B:241:LYS:HD3	2.29	0.47
1:B:81:PRO:HA	1:B:82:PRO:HD3	1.71	0.47
1:A:122:TYR:CZ	1:A:176:GLU:HB3	2.49	0.47
1:A:218:LEU:C	1:A:220:ILE:N	2.67	0.47
1:B:43:GLY:O	1:B:44:LEU:O	2.32	0.47
1:A:109:LEU:CD2	1:A:184:LEU:HD13	2.43	0.47
1:A:204:LEU:HD12	1:A:267:LEU:CD2	2.43	0.47
1:B:23:GLY:C	1:B:25:ASP:N	2.67	0.47
1:A:28:LYS:O	1:A:32:GLU:HG2	2.14	0.47
1:A:24:GLN:NE2	1:A:46:ILE:H	2.11	0.47
1:C:169:THR:N	1:C:172:GLN:HE21	2.13	0.47
1:B:139:ASP:CA	1:B:159:MET:HE1	2.44	0.47
1:B:124:ILE:HG23	1:B:128:LEU:HD12	1.95	0.47
1:A:44:LEU:N	1:A:77:VAL:HA	2.29	0.47
1:A:228:VAL:HA	1:A:242:ILE:HG22	1.97	0.47
1:A:169:THR:OG1	1:A:172:GLN:HG3	2.15	0.47
1:B:242:ILE:HG12	1:B:243:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ARG:O	1:C:261:TYR:HA	2.15	0.47
1:B:36:LEU:O	1:B:36:LEU:CD1	2.63	0.47
1:B:139:ASP:HA	1:B:159:MET:HE1	1.96	0.47
1:C:276:THR:O	1:C:279:ARG:HB2	2.15	0.47
1:C:230:LYS:N	1:C:242:ILE:HD11	2.29	0.47
1:A:186:MET:HE3	1:A:214:TYR:CE1	2.50	0.47
1:A:186:MET:CE	1:A:214:TYR:OH	2.63	0.47
1:B:47:TRP:CD2	1:B:53:LYS:HB3	2.50	0.47
1:B:51:THR:HG22	1:B:52:SER:H	1.80	0.47
1:B:37:LEU:HD13	1:B:44:LEU:HG	1.96	0.47
1:A:45:ALA:HB3	1:A:78:LYS:HB2	1.96	0.47
1:B:227:LYS:HZ1	1:B:245:GLY:HA2	1.79	0.47
1:C:225:TRP:O	1:C:226:PRO:C	2.53	0.46
1:A:262:ARG:HE	1:C:36:LEU:HD13	1.78	0.46
1:C:115:THR:C	1:C:117:ALA:N	2.68	0.46
1:C:38:GLU:OE1	1:C:38:GLU:HA	2.15	0.46
1:C:182:LYS:HD2	1:C:183:LYS:HE3	1.95	0.46
1:C:97:CYS:O	1:C:101:ARG:HG3	2.15	0.46
1:C:247:GLN:HG2	1:C:247:GLN:O	2.15	0.46
1:B:86:GLN:O	1:B:86:GLN:HG3	2.16	0.46
1:B:49:ASN:HD22	1:B:49:ASN:N	2.11	0.46
1:C:139:ASP:O	1:C:142:SER:N	2.49	0.46
1:B:186:MET:HE2	1:B:189:VAL:HG21	1.97	0.46
1:A:248:GLU:O	1:A:249:GLN:HB2	2.15	0.46
1:A:212:LEU:HB2	1:A:214:TYR:HE2	1.80	0.46
1:B:131:TYR:O	1:B:132:ASP:O	2.34	0.46
1:B:130:ASP:OD1	1:B:166:ARG:HA	2.16	0.46
1:A:95:TYR:OH	1:B:67:ARG:CZ	2.64	0.46
1:A:243:ARG:HH22	1:A:248:GLU:HA	1.80	0.46
1:A:215:LYS:HG2	1:A:216:ASP:OD2	2.15	0.46
1:B:76:ASN:HD22	1:B:99:GLN:HE22	1.63	0.46
1:C:47:TRP:CE3	1:C:53:LYS:HA	2.50	0.46
1:C:124:ILE:HD11	1:C:141:VAL:HG13	1.98	0.46
1:B:244:PRO:HA	1:B:250:TYR:O	2.16	0.46
1:B:279:ARG:HH11	1:B:279:ARG:HG2	1.79	0.46
1:A:43:GLY:C	1:A:77:VAL:HA	2.36	0.45
1:C:230:LYS:N	1:C:242:ILE:CD1	2.79	0.45
1:B:279:ARG:HD3	1:B:279:ARG:H	1.81	0.45
1:C:41:TYR:O	1:C:42:PHE:C	2.55	0.45
1:C:116:LEU:HD21	1:C:147:ALA:HB1	1.98	0.45
1:A:211:LEU:C	1:A:212:LEU:HD23	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:H	1:B:26:LEU:CD1	2.28	0.45
1:A:230:LYS:HZ2	1:A:241:LYS:HZ2	1.64	0.45
1:A:225:TRP:C	1:A:227:LYS:N	2.69	0.45
1:A:134:GLU:HG2	1:A:135:LEU:CD1	2.46	0.45
1:A:23:GLY:C	1:A:25:ASP:N	2.70	0.45
1:A:47:TRP:HZ3	1:A:49:ASN:CA	2.29	0.45
1:B:250:TYR:HE1	1:B:252:SER:CB	2.29	0.45
1:A:198:GLU:HB3	1:A:200:VAL:HG22	1.98	0.45
1:A:43:GLY:O	1:A:78:LYS:N	2.44	0.45
1:A:47:TRP:NE1	1:A:76:ASN:CG	2.70	0.45
1:A:204:LEU:CD1	1:A:267:LEU:HD21	2.44	0.45
1:B:44:LEU:HD13	1:B:77:VAL:HG22	1.99	0.45
1:C:202:ILE:C	1:C:202:ILE:HD12	2.36	0.45
1:C:115:THR:O	1:C:117:ALA:N	2.50	0.45
1:A:130:ASP:OD1	1:A:167:SER:N	2.41	0.45
1:B:28:LYS:HZ2	1:B:28:LYS:HB3	1.72	0.45
1:B:47:TRP:NE1	1:B:76:ASN:OD1	2.50	0.45
1:C:229:LEU:H	1:C:242:ILE:CG1	2.30	0.45
1:C:238:PHE:HB2	1:C:258:LEU:HD12	1.99	0.45
1:C:175:LEU:C	1:C:175:LEU:HD13	2.37	0.45
1:B:191:LEU:HD22	1:B:203:ILE:CG2	2.47	0.45
1:A:246:GLU:OE1	1:A:246:GLU:HA	2.17	0.45
1:C:195:LYS:HG3	1:C:201:ASP:HA	1.98	0.45
1:C:77:VAL:HB	1:C:99:GLN:HG2	1.98	0.45
1:C:130:ASP:OD1	1:C:167:SER:N	2.49	0.45
1:B:66:VAL:HB	1:B:69:VAL:HG23	1.98	0.45
1:A:210:GLY:HA2	1:A:225:TRP:NE1	2.30	0.44
1:C:125:GLN:HG3	1:C:168:MET:HE1	1.97	0.44
1:B:57:ASP:OD1	1:B:59:ALA:N	2.50	0.44
1:C:44:LEU:HD12	1:C:75:PHE:CZ	2.51	0.44
1:A:131:TYR:HE2	1:A:133:PRO:HG3	1.82	0.44
1:B:32:GLU:CA	1:B:32:GLU:OE2	2.65	0.44
1:A:243:ARG:HA	1:A:244:PRO:HD3	1.77	0.44
1:B:209:SER:HB3	1:B:222:ARG:NH2	2.32	0.44
1:A:137:GLY:C	1:A:139:ASP:H	2.20	0.44
1:C:138:VAL:O	1:C:138:VAL:HG12	2.18	0.44
1:C:155:GLU:O	1:C:159:MET:HG3	2.17	0.44
1:A:219:ARG:HB3	1:A:219:ARG:CZ	2.47	0.44
1:A:41:TYR:CD2	1:A:41:TYR:N	2.85	0.44
1:A:211:LEU:HB3	1:A:223:PHE:HD1	1.83	0.44
1:C:124:ILE:HG12	1:C:141:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:VAL:CG1	1:C:141:VAL:O	2.65	0.44
1:C:9:ASP:O	1:C:10:ASP:HB2	2.16	0.44
1:B:77:VAL:N	1:B:99:GLN:HE21	2.03	0.44
1:A:24:GLN:O	1:A:25:ASP:C	2.56	0.44
1:A:186:MET:HE3	1:A:214:TYR:OH	2.17	0.44
1:B:213:VAL:CG2	1:B:221:ASN:HB2	2.47	0.44
1:A:195:LYS:HA	1:A:200:VAL:O	2.17	0.44
1:B:131:TYR:O	1:B:135:LEU:HD13	2.17	0.44
1:B:165:TYR:CD1	1:B:168:MET:HE1	2.53	0.44
1:C:21:ALA:CB	1:C:26:LEU:HD12	2.46	0.44
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.90	0.44
1:A:36:LEU:HD21	1:B:262:ARG:HG3	1.99	0.44
1:C:196:ASP:N	1:C:200:VAL:O	2.48	0.44
1:C:192:HIS:CD2	1:C:267:LEU:HD13	2.53	0.44
1:B:125:GLN:NE2	1:B:162:HIS:CE1	2.86	0.44
1:C:157:LYS:O	1:C:161:LEU:HB2	2.18	0.44
1:A:24:GLN:C	1:A:26:LEU:N	2.70	0.43
1:C:138:VAL:CG1	1:C:159:MET:HE3	2.48	0.43
1:B:152:LYS:HA	1:B:155:GLU:OE1	2.18	0.43
1:B:141:VAL:H	1:B:159:MET:HE2	1.83	0.43
1:A:68:GLY:O	1:A:69:VAL:HG23	2.18	0.43
1:B:24:GLN:HA	1:B:28:LYS:H	1.83	0.43
1:A:217:LYS:O	1:A:218:LEU:C	2.56	0.43
1:C:145:LYS:HA	1:C:150:GLN:OE1	2.18	0.43
1:C:196:ASP:O	1:C:199:GLY:N	2.52	0.43
1:C:28:LYS:O	1:C:32:GLU:HG2	2.18	0.43
1:C:125:GLN:HG3	1:C:168:MET:HE2	1.97	0.43
1:B:25:ASP:O	1:B:29:ARG:HB2	2.17	0.43
1:B:144:PHE:O	1:B:150:GLN:OE1	2.35	0.43
1:B:149:ASN:HD22	1:B:151:THR:HG23	1.83	0.43
1:A:262:ARG:NH2	1:C:36:LEU:HD13	2.33	0.43
1:A:235:ARG:HG2	1:A:235:ARG:NH1	2.33	0.43
1:A:139:ASP:HA	1:A:159:MET:HE1	2.00	0.43
1:C:218:LEU:HD22	1:C:218:LEU:N	2.33	0.43
1:C:162:HIS:HA	1:C:165:TYR:CD1	2.54	0.43
1:C:278:PHE:O	1:C:279:ARG:C	2.56	0.43
1:A:37:LEU:HD13	1:A:44:LEU:HG	2.00	0.43
1:C:219:ARG:NH1	1:C:222:ARG:HB2	2.24	0.43
1:C:145:LYS:HE2	1:C:145:LYS:HB2	1.86	0.43
1:B:208:SER:HA	1:B:278:PHE:CD1	2.54	0.43
1:B:147:ALA:HB1	1:B:148:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TYR:CD1	1:A:34:LEU:HG	2.53	0.43
1:C:151:THR:O	1:C:154:LEU:N	2.44	0.43
1:B:113:PHE:C	1:B:113:PHE:CD2	2.91	0.43
1:C:30:VAL:O	1:C:33:HIS:HB2	2.19	0.43
1:C:162:HIS:HA	1:C:165:TYR:HD1	1.84	0.43
1:C:256:PHE:N	1:C:256:PHE:CD1	2.86	0.43
1:A:159:MET:O	1:A:163:LYS:HG3	2.19	0.43
1:C:235:ARG:HB3	1:C:236:SER:H	1.61	0.43
1:C:244:PRO:HB2	1:C:247:GLN:HE21	1.84	0.43
1:A:27:LEU:O	1:A:30:VAL:HB	2.18	0.43
1:A:3:CYS:SG	1:A:17:VAL:HG22	2.58	0.43
1:A:23:GLY:O	1:A:24:GLN:C	2.56	0.43
1:A:96:LEU:O	1:A:100:LEU:HG	2.19	0.43
1:A:46:ILE:HG22	1:A:75:PHE:HA	2.00	0.42
1:B:244:PRO:HG2	1:B:248:GLU:CA	2.45	0.42
1:C:80:TYR:CD1	1:C:188:GLY:HA2	2.54	0.42
1:B:202:ILE:HD11	1:B:256:PHE:CD2	2.54	0.42
1:B:46:ILE:HG22	1:B:74:THR:O	2.19	0.42
1:C:172:GLN:O	1:C:173:ALA:C	2.57	0.42
1:A:141:VAL:C	1:A:143:ASP:H	2.23	0.42
1:A:230:LYS:NZ	1:A:241:LYS:NZ	2.67	0.42
1:A:117:ALA:HB2	1:A:154:LEU:CD2	2.50	0.42
1:A:60:LYS:O	1:A:61:GLU:C	2.58	0.42
1:A:44:LEU:H	1:A:44:LEU:HD13	1.84	0.42
1:C:219:ARG:NH1	1:C:219:ARG:HB3	2.34	0.42
1:A:136:HIS:O	1:A:137:GLY:O	2.37	0.42
1:C:93:ARG:HB3	1:C:178:LEU:HD11	2.02	0.42
1:C:177:PHE:C	1:C:177:PHE:CD1	2.92	0.42
1:A:243:ARG:CZ	1:A:244:PRO:HD2	2.50	0.42
1:C:134:GLU:C	1:C:136:HIS:H	2.22	0.42
1:C:78:LYS:HD3	1:C:79:PHE:CE1	2.54	0.42
1:C:99:GLN:O	1:C:102:GLN:HB3	2.19	0.42
1:C:125:GLN:HE22	1:C:130:ASP:HA	1.84	0.42
1:C:186:MET:HE2	1:C:189:VAL:HG11	2.02	0.42
1:B:234:LYS:O	1:B:235:ARG:HB2	2.19	0.42
1:A:230:LYS:NZ	1:A:241:LYS:HZ2	2.18	0.42
1:C:165:TYR:HB3	1:C:168:MET:HE2	2.00	0.42
1:A:215:LYS:C	1:A:217:LYS:H	2.23	0.42
1:A:141:VAL:O	1:A:143:ASP:N	2.52	0.42
1:A:247:GLN:HG3	1:A:250:TYR:CD2	2.54	0.42
1:A:44:LEU:HD13	1:A:77:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HD11	1:A:238:PHE:HE2	1.84	0.42
1:A:262:ARG:NE	1:C:36:LEU:HD11	2.35	0.41
1:C:151:THR:O	1:C:152:LYS:C	2.58	0.41
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.80	0.41
1:C:243:ARG:HA	1:C:243:ARG:NE	2.35	0.41
1:C:55:TRP:CE2	1:C:78:LYS:HG3	2.54	0.41
1:A:215:LYS:O	1:A:216:ASP:HB2	2.21	0.41
1:C:247:GLN:CG	1:C:250:TYR:HD2	2.32	0.41
1:B:47:TRP:CD2	1:B:53:LYS:CB	3.03	0.41
1:B:194:ALA:HB2	1:B:258:LEU:HD23	2.01	0.41
1:C:225:TRP:O	1:C:228:VAL:HB	2.20	0.41
1:B:151:THR:O	1:B:154:LEU:HB3	2.20	0.41
1:C:132:ASP:OD1	1:C:132:ASP:C	2.59	0.41
1:A:229:LEU:H	1:A:242:ILE:CG2	2.33	0.41
1:C:189:VAL:CG2	1:C:207:CYS:HB3	2.50	0.41
1:A:115:THR:HG21	1:A:184:LEU:HD21	2.01	0.41
1:B:45:ALA:HB3	1:B:78:LYS:HB2	2.02	0.41
1:A:131:TYR:O	1:A:132:ASP:HB3	2.21	0.41
1:C:116:LEU:HG	1:C:116:LEU:O	2.21	0.41
1:C:144:PHE:O	1:C:150:GLN:OE1	2.38	0.41
1:B:93:ARG:HB3	1:B:178:LEU:HD11	2.02	0.41
1:B:32:GLU:HA	1:B:32:GLU:OE2	2.20	0.41
1:B:204:LEU:HD12	1:B:267:LEU:CD2	2.46	0.41
1:B:279:ARG:H	1:B:279:ARG:CD	2.33	0.41
1:B:32:GLU:OE2	1:B:75:PHE:HE2	2.04	0.41
1:B:24:GLN:CB	1:B:28:LYS:HZ2	2.20	0.41
1:A:47:TRP:HD1	1:A:55:TRP:CZ3	2.38	0.41
1:A:243:ARG:CA	1:A:243:ARG:NE	2.83	0.41
1:A:244:PRO:CB	1:A:247:GLN:NE2	2.80	0.41
1:C:200:VAL:O	1:C:202:ILE:HG13	2.21	0.41
1:C:241:LYS:CB	1:C:253:THR:HA	2.50	0.41
1:C:42:PHE:O	1:C:43:GLY:C	2.59	0.41
1:C:69:VAL:HG13	1:C:70:PRO:HD2	2.03	0.41
1:B:43:GLY:HA2	1:B:78:LYS:CA	2.49	0.41
1:B:197:LEU:C	1:B:199:GLY:H	2.24	0.41
1:C:202:ILE:HB	1:C:214:TYR:O	2.20	0.40
1:C:24:GLN:O	1:C:26:LEU:N	2.54	0.40
1:B:145:LYS:CD	1:B:145:LYS:H	2.33	0.40
1:A:262:ARG:HG3	1:C:36:LEU:HD21	2.03	0.40
1:A:121:SER:HA	1:A:158:VAL:HG13	2.03	0.40
1:B:137:GLY:C	1:B:139:ASP:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:O	1:A:257:LYS:HG3	2.21	0.40
1:C:43:GLY:HA2	1:C:78:LYS:N	2.32	0.40
1:C:43:GLY:HA2	1:C:79:PHE:N	2.18	0.40
1:A:225:TRP:O	1:A:227:LYS:N	2.54	0.40
1:A:149:ASN:ND2	1:A:150:GLN:N	2.68	0.40
1:A:175:LEU:O	1:A:179:GLU:HG2	2.21	0.40
1:B:113:PHE:O	1:B:114:ALA:CB	2.69	0.40
1:A:89:GLU:OE1	1:A:91:ILE:HD11	2.21	0.40
1:C:41:TYR:O	1:C:43:GLY:N	2.53	0.40
1:A:215:LYS:O	1:A:216:ASP:CB	2.69	0.40
1:C:196:ASP:O	1:C:198:GLU:N	2.55	0.40
1:C:156:GLU:O	1:C:158:VAL:N	2.55	0.40
1:C:208:SER:HA	1:C:278:PHE:CD1	2.57	0.40
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.88	0.40

All (2) 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:B:251:GLU:OE1	1:B:251:GLU:OE1[2_656]	1.67	0.53
1:C:197:LEU:CD1	1:C:197:LEU:CD1[2_556]	1.68	0.52

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	277/279 (99%)	217 (78%)	36 (13%)	24 (9%)	1 2
1	B	277/279 (99%)	235 (85%)	27 (10%)	15 (5%)	2 7
1	C	277/279 (99%)	209 (76%)	43 (16%)	25 (9%)	1 2
All	All	831/837 (99%)	661 (80%)	106 (13%)	64 (8%)	1 2

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ALA
1	A	136	HIS
1	A	198	GLU
1	A	220	ILE
1	A	242	ILE
1	A	243	ARG
1	B	43	GLY
1	B	49	ASN
1	B	114	ALA
1	B	137	GLY
1	B	150	GLN
1	B	244	PRO
1	C	24	GLN
1	C	49	ASN
1	C	131	TYR
1	C	136	HIS
1	C	140	TYR
1	C	198	GLU
1	A	23	GLY
1	A	24	GLN
1	A	43	GLY
1	A	131	TYR
1	A	137	GLY
1	A	139	ASP
1	A	142	SER
1	A	197	LEU
1	A	218	LEU
1	B	24	GLN
1	B	44	LEU
1	B	131	TYR
1	B	132	ASP
1	B	136	HIS
1	B	218	LEU
1	C	23	GLY
1	C	132	ASP
1	C	137	GLY
1	C	197	LEU
1	C	218	LEU
1	C	242	ILE
1	C	247	GLN
1	A	44	LEU
1	A	132	ASP

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Mol	Chain	Res	Type
1	A	248	GLU
1	A	252	SER
1	B	138	VAL
1	C	42	PHE
1	C	150	GLN
1	A	25	ASP
1	A	42	PHE
1	A	130	ASP
1	A	138	VAL
1	C	116	LEU
1	C	252	SER
1	A	217	LYS
1	B	41	TYR
1	C	118	LEU
1	C	186	MET
1	C	227	LYS
1	C	243	ARG
1	C	50	ALA
1	B	243	ARG
1	C	200	VAL
1	C	220	ILE
1	C	202	ILE

5.3.2 Protein sidechains ⓘ

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	251/251 (100%)	228 (91%)	23 (9%)	11	32
1	B	251/251 (100%)	222 (88%)	29 (12%)	7	20
1	C	251/251 (100%)	226 (90%)	25 (10%)	9	27
All	All	753/753 (100%)	676 (90%)	77 (10%)	9	26

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	LEU
1	A	36	LEU
1	A	38	GLU
1	A	40	ASP
1	A	44	LEU
1	A	46	ILE
1	A	48	ASP
1	A	56	LEU
1	A	90	ASP
1	A	91	ILE
1	A	96	LEU
1	A	109	LEU
1	A	118	LEU
1	A	154	LEU
1	A	175	LEU
1	A	196	ASP
1	A	200	VAL
1	A	211	LEU
1	A	212	LEU
1	A	221	ASN
1	A	222	ARG
1	A	257	LYS
1	B	18	GLU
1	B	27	LEU
1	B	33	HIS
1	B	34	LEU
1	B	36	LEU
1	B	40	ASP
1	B	44	LEU
1	B	49	ASN
1	B	58	SER
1	B	65	GLN
1	B	91	ILE
1	B	102	GLN
1	B	109	LEU
1	B	113	PHE
1	B	116	LEU
1	B	118	LEU
1	B	126	SER
1	B	145	LYS
1	B	150	GLN
1	B	154	LEU

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Mol	Chain	Res	Type
1	B	164	SER
1	B	182	LYS
1	B	201	ASP
1	B	211	LEU
1	B	232	SER
1	B	241	LYS
1	B	242	ILE
1	B	250	TYR
1	B	279	ARG
1	C	18	GLU
1	C	27	LEU
1	C	34	LEU
1	C	36	LEU
1	C	38	GLU
1	C	44	LEU
1	C	48	ASP
1	C	49	ASN
1	C	54	THR
1	C	56	LEU
1	C	91	ILE
1	C	96	LEU
1	C	109	LEU
1	C	115	THR
1	C	118	LEU
1	C	135	LEU
1	C	145	LYS
1	C	150	GLN
1	C	154	LEU
1	C	195	LYS
1	C	211	LEU
1	C	222	ARG
1	C	227	LYS
1	C	234	LYS
1	C	257	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	65	GLN
1	A	102	GLN
1	A	125	GLN

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Mol	Chain	Res	Type
1	A	136	HIS
1	A	149	ASN
1	A	162	HIS
1	A	172	GLN
1	A	247	GLN
1	A	274	HIS
1	B	33	HIS
1	B	49	ASN
1	B	65	GLN
1	B	99	GLN
1	B	125	GLN
1	B	162	HIS
1	B	172	GLN
1	B	247	GLN
1	C	65	GLN
1	C	162	HIS
1	C	172	GLN
1	C	192	HIS

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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