



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:01 PM UTC

PDB ID : 1AV1 / pdb_00001av1
Title : CRYSTAL STRUCTURE OF HUMAN APOLIPOPROTEIN A-I
Authors : Borhani, D.W.; Rogers, D.P.; Engler, J.A.; Brouillette, C.G.
Deposited on : 1997-09-23
Resolution : 4.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

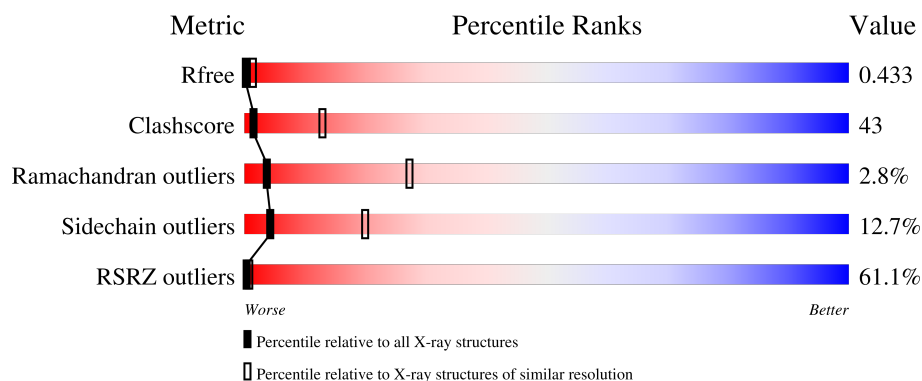
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	201	64% 32% 55% 11%
1	B	201	57% 34% 52% 13%
1	C	201	66% 33% 54% 11%
1	D	201	57% 32% 54% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6588 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.

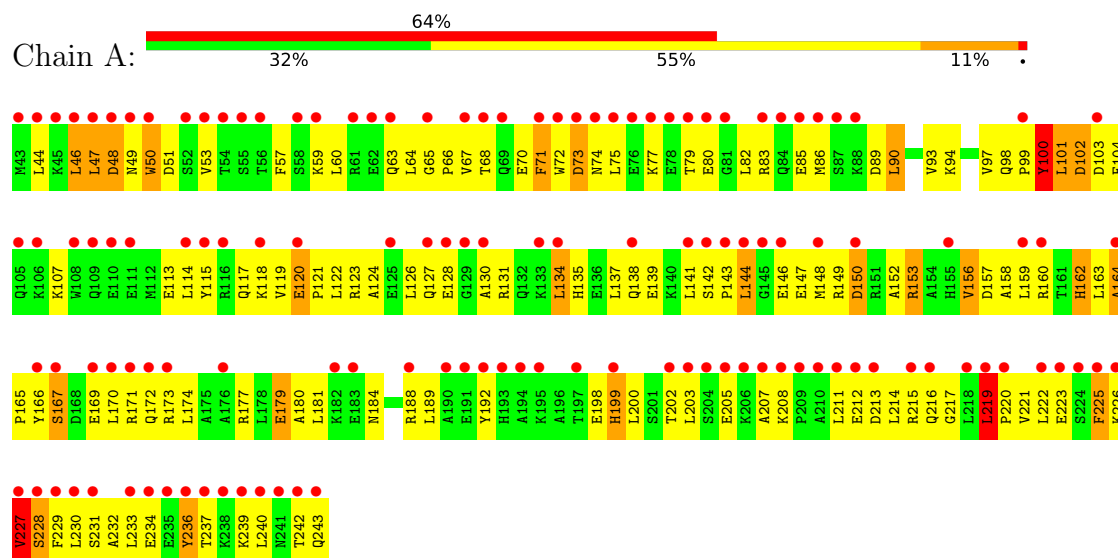
- Molecule 1 is a protein called APOLIPOPROTEIN A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1647	1033	291	319	4			
1	B	201	Total	C	N	O	S	0	0	0
			1647	1033	291	319	4			
1	C	201	Total	C	N	O	S	0	0	0
			1647	1033	291	319	4			
1	D	201	Total	C	N	O	S	0	0	0
			1647	1033	291	319	4			

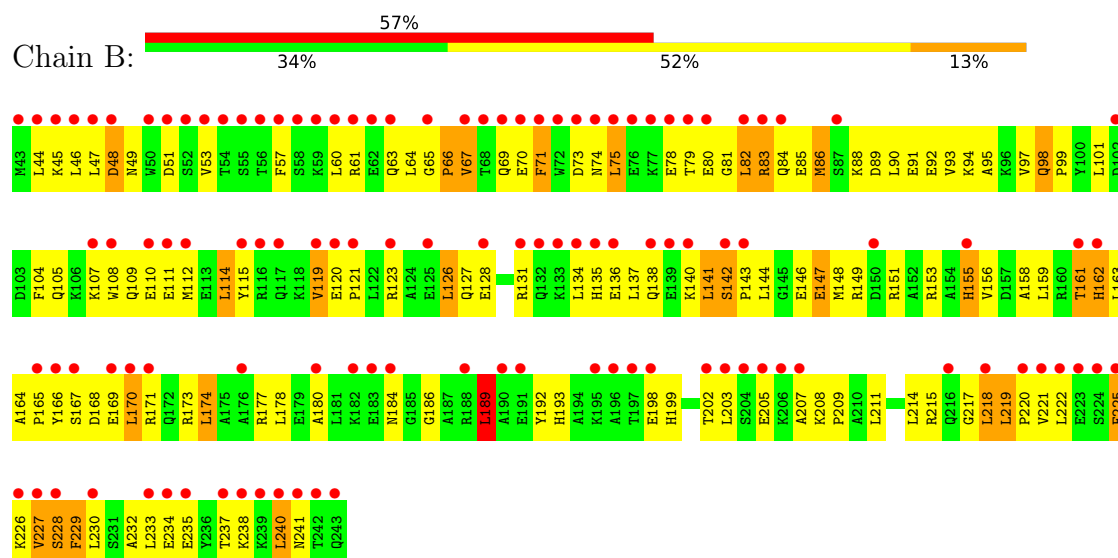
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: APOLIPOPROTEIN A-I

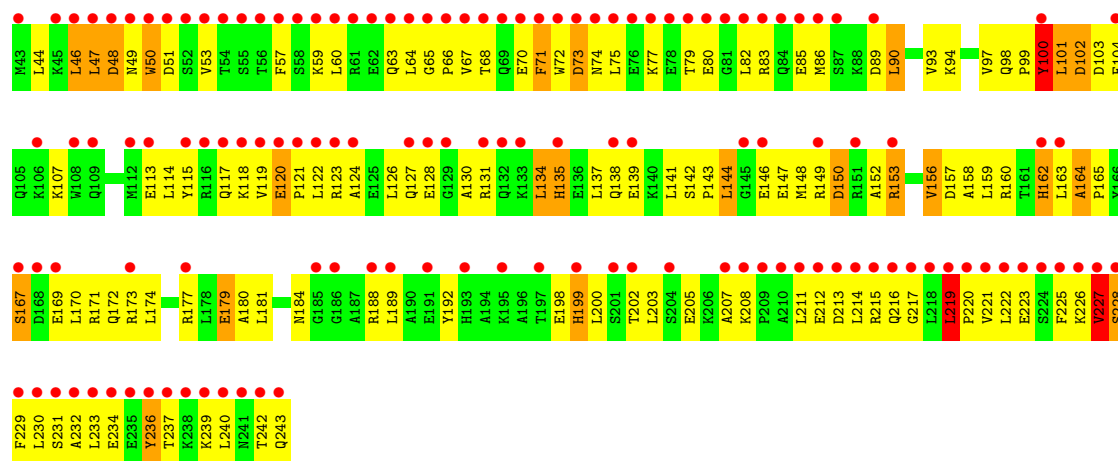


• Molecule 1: APOLIPOPROTEIN A-I

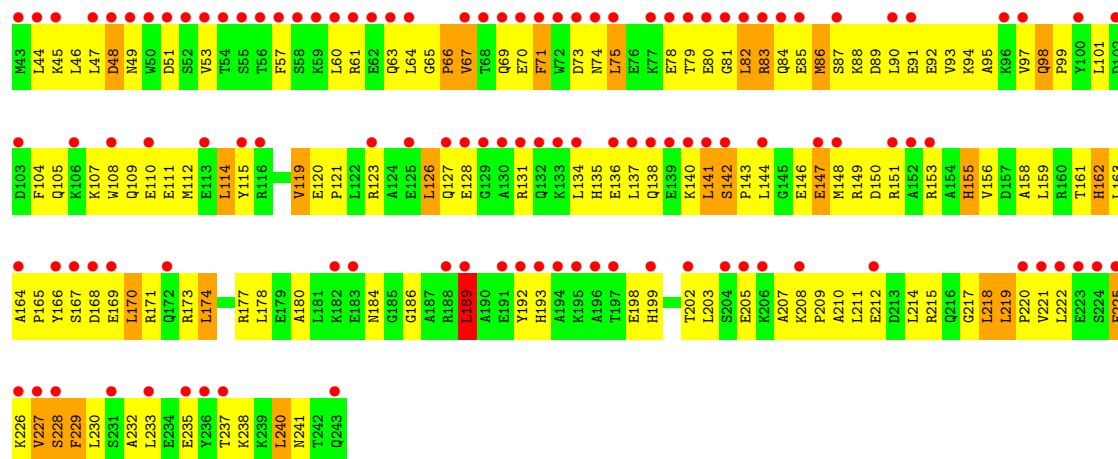


• Molecule 1: APOLIPOPROTEIN A-I





● Molecule 1: APOLIPOPROTEIN A-I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.47Å 113.87Å 196.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.00 – 4.00 27.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	81.8 (27.00-4.00) 84.9 (27.00-4.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.98Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.382 , 0.428 0.399 , 0.433	Depositor DCC
R_{free} test set	822 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 94.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	6588	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/1674	1.04	12/2250 (0.5%)
1	B	0.67	0/1674	1.10	10/2250 (0.4%)
1	C	0.66	0/1674	1.04	12/2250 (0.5%)
1	D	0.67	0/1674	1.10	10/2250 (0.4%)
All	All	0.66	0/6696	1.07	44/9000 (0.5%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	VAL	N-CA-C	-9.71	101.10	110.42
1	D	67	VAL	N-CA-C	-9.69	101.12	110.42
1	B	219	LEU	CA-C-N	7.04	128.64	119.84
1	B	219	LEU	C-N-CA	7.04	128.64	119.84
1	D	219	LEU	CA-C-N	7.03	128.62	119.84
1	D	219	LEU	C-N-CA	7.03	128.62	119.84
1	D	119	VAL	CB-CA-C	-6.94	104.84	111.44
1	B	119	VAL	CB-CA-C	-6.94	104.85	111.44
1	A	167	SER	N-CA-C	-6.51	103.08	111.02
1	C	167	SER	N-CA-C	-6.51	103.08	111.02
1	D	225	PHE	N-CA-C	6.40	118.84	108.34
1	B	225	PHE	N-CA-C	6.39	118.83	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	VAL	N-CA-C	6.05	116.77	111.56
1	D	119	VAL	N-CA-C	6.04	116.76	111.56
1	D	189	LEU	N-CA-C	-5.86	104.81	111.14
1	B	189	LEU	N-CA-C	-5.83	104.84	111.14
1	A	212	GLU	N-CA-C	-5.80	106.04	113.23
1	C	212	GLU	N-CA-C	-5.79	106.05	113.23
1	A	82	LEU	N-CA-C	-5.79	106.38	113.50
1	C	82	LEU	N-CA-C	-5.78	106.39	113.50
1	C	179	GLU	N-CA-C	-5.70	105.21	111.82
1	C	120	GLU	CA-C-N	5.69	125.06	118.85
1	C	120	GLU	C-N-CA	5.69	125.06	118.85
1	A	179	GLU	N-CA-C	-5.69	105.22	111.82
1	A	120	GLU	CA-C-N	5.66	125.02	118.85
1	A	120	GLU	C-N-CA	5.66	125.02	118.85
1	D	228	SER	N-CA-C	-5.63	105.14	111.28
1	B	228	SER	N-CA-C	-5.62	105.15	111.28
1	D	83	ARG	N-CA-C	-5.58	104.57	111.33
1	B	83	ARG	N-CA-C	-5.57	104.59	111.33
1	B	82	LEU	N-CA-C	-5.56	105.62	112.90
1	D	82	LEU	N-CA-C	-5.55	105.62	112.90
1	A	156	VAL	CB-CA-C	-5.54	104.88	111.81
1	C	156	VAL	CB-CA-C	-5.54	104.88	111.81
1	A	50	TRP	N-CA-C	-5.52	105.18	111.14
1	C	50	TRP	N-CA-C	-5.51	105.19	111.14
1	C	46	LEU	N-CA-C	-5.38	106.67	113.18
1	A	46	LEU	N-CA-C	-5.35	106.71	113.18
1	A	48	ASP	N-CA-C	-5.25	107.17	113.21
1	C	100	TYR	CA-CB-CG	-5.23	104.48	113.90
1	C	48	ASP	N-CA-C	-5.23	107.20	113.21
1	A	100	TYR	CA-CB-CG	-5.22	104.50	113.90
1	C	53	VAL	N-CA-C	5.10	115.77	110.82
1	A	53	VAL	N-CA-C	5.09	115.75	110.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain
1	C	100	TYR	Sidechain

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	1647	0	1650	180	14
1	B	1647	0	1650	175	24
1	C	1647	0	1650	175	23
1	D	1647	0	1650	179	16
All	All	6588	0	6600	571	40

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 43.

All (571) 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:66:PRO:HA	1:B:69:GLN:HB3	1.39	1.03
1:D:66:PRO:HA	1:D:69:GLN:HB3	1.40	1.01
1:A:134:LEU:HD22	1:D:233:LEU:HD13	1.48	0.94
1:B:171:ARG:HE	1:C:215:ARG:HB2	1.35	0.92
1:B:148:MET:HA	1:B:151:ARG:HB2	1.53	0.91
1:D:137:LEU:O	1:D:141:LEU:HB3	1.73	0.88
1:B:137:LEU:O	1:B:141:LEU:HB3	1.73	0.88
1:D:148:MET:HA	1:D:151:ARG:HB2	1.53	0.87
1:B:233:LEU:HD13	1:C:134:LEU:HD22	1.56	0.86
1:C:216:GLN:O	1:C:220:PRO:HD2	1.76	0.86
1:A:93:VAL:HG21	1:B:170:LEU:HD11	1.59	0.85
1:B:49:ASN:ND2	1:C:94:LYS:HE3	1.91	0.85
1:A:216:GLN:O	1:A:220:PRO:HD2	1.76	0.85
1:C:93:VAL:HG21	1:D:170:LEU:HD11	1.58	0.84
1:D:227:VAL:HG23	1:D:230:LEU:H	1.43	0.83
1:C:142:SER:N	1:C:143:PRO:HD2	1.94	0.83
1:C:207:ALA:O	1:C:211:LEU:HG	1.79	0.82
1:A:143:PRO:HG2	1:A:144:LEU:HD13	1.61	0.82
1:A:142:SER:N	1:A:143:PRO:HD2	1.94	0.82
1:B:227:VAL:HG23	1:B:230:LEU:H	1.43	0.81
1:C:143:PRO:HG2	1:C:144:LEU:HD13	1.61	0.81
1:A:207:ALA:O	1:A:211:LEU:HG	1.79	0.81
1:A:215:ARG:HB2	1:D:171:ARG:HE	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HD11	1:C:127:GLN:HA	1.64	0.80
1:B:171:ARG:HH21	1:C:215:ARG:H	1.27	0.79
1:B:208:LYS:HA	1:B:211:LEU:HD12	1.64	0.79
1:D:208:LYS:HA	1:D:211:LEU:HD12	1.64	0.79
1:B:159:LEU:HA	1:B:162:HIS:HB2	1.65	0.79
1:B:98:GLN:HE21	1:B:98:GLN:HA	1.48	0.79
1:D:98:GLN:HA	1:D:98:GLN:HE21	1.48	0.78
1:A:65:GLY:N	1:A:66:PRO:HD2	2.00	0.77
1:D:159:LEU:HA	1:D:162:HIS:HB2	1.65	0.77
1:C:192:TYR:OH	1:D:67:VAL:HG22	1.85	0.76
1:D:126:LEU:HD23	1:D:127:GLN:N	2.00	0.76
1:A:192:TYR:OH	1:B:67:VAL:HG22	1.85	0.76
1:C:65:GLY:N	1:C:66:PRO:HD2	2.00	0.76
1:B:126:LEU:HD23	1:B:127:GLN:N	2.00	0.76
1:B:171:ARG:NH2	1:C:215:ARG:H	1.84	0.76
1:A:93:VAL:HG11	1:B:170:LEU:HD21	1.69	0.75
1:A:202:THR:O	1:A:205:GLU:HG3	1.86	0.75
1:C:202:THR:O	1:C:205:GLU:HG3	1.86	0.75
1:A:94:LYS:HE3	1:D:49:ASN:ND2	2.02	0.75
1:D:146:GLU:HA	1:D:149:ARG:HB3	1.68	0.75
1:A:94:LYS:HE2	1:D:46:LEU:HB2	1.68	0.74
1:C:93:VAL:HG11	1:D:170:LEU:HD21	1.69	0.73
1:C:227:VAL:CG1	1:C:230:LEU:HB3	2.19	0.73
1:A:227:VAL:CG1	1:A:230:LEU:HB3	2.19	0.73
1:A:227:VAL:HG11	1:A:230:LEU:HB3	1.71	0.73
1:B:146:GLU:HA	1:B:149:ARG:HB3	1.68	0.73
1:A:137:LEU:O	1:A:141:LEU:HG	1.89	0.72
1:C:227:VAL:HG11	1:C:230:LEU:HB3	1.71	0.72
1:C:137:LEU:O	1:C:141:LEU:HG	1.89	0.72
1:D:214:LEU:O	1:D:218:LEU:HD13	1.91	0.71
1:B:70:GLU:O	1:B:74:ASN:HB2	1.91	0.71
1:B:222:LEU:CD2	1:C:156:VAL:HG11	2.21	0.71
1:C:237:THR:HA	1:C:240:LEU:HG	1.72	0.71
1:D:70:GLU:O	1:D:74:ASN:HB2	1.91	0.71
1:A:127:GLN:HA	1:D:240:LEU:HD11	1.73	0.71
1:A:215:ARG:H	1:D:171:ARG:HH21	1.37	0.70
1:C:146:GLU:O	1:C:150:ASP:HB2	1.91	0.70
1:A:146:GLU:O	1:A:150:ASP:HB2	1.91	0.70
1:B:214:LEU:O	1:B:218:LEU:HD13	1.91	0.70
1:A:237:THR:HA	1:A:240:LEU:HG	1.72	0.70
1:B:46:LEU:HB2	1:C:94:LYS:HE2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:O	1:D:134:LEU:HB3	1.92	0.69
1:C:71:PHE:O	1:C:75:LEU:HG	1.93	0.69
1:A:44:LEU:HD22	1:B:217:GLY:O	1.93	0.69
1:B:211:LEU:O	1:B:214:LEU:HB3	1.93	0.69
1:B:131:ARG:O	1:B:134:LEU:HB3	1.92	0.69
1:C:44:LEU:HD22	1:D:217:GLY:O	1.93	0.69
1:C:221:VAL:HG11	1:D:45:LYS:HG2	1.75	0.69
1:C:122:LEU:O	1:C:126:LEU:HG	1.94	0.68
1:D:211:LEU:O	1:D:214:LEU:HB3	1.93	0.68
1:A:71:PHE:O	1:A:75:LEU:HG	1.93	0.68
1:B:203:LEU:HD21	1:C:181:LEU:HD23	1.75	0.68
1:A:221:VAL:HG11	1:B:45:LYS:HG2	1.75	0.67
1:C:180:ALA:O	1:C:184:ASN:HB2	1.95	0.67
1:A:180:ALA:O	1:A:184:ASN:HB2	1.95	0.67
1:B:98:GLN:N	1:B:99:PRO:HD2	2.09	0.67
1:D:98:GLN:N	1:D:99:PRO:HD2	2.09	0.67
1:A:122:LEU:O	1:A:126:LEU:HG	1.94	0.67
1:A:181:LEU:HD23	1:D:203:LEU:HD21	1.76	0.66
1:C:44:LEU:HD13	1:D:218:LEU:O	1.96	0.65
1:A:44:LEU:HD21	1:B:219:LEU:O	1.97	0.65
1:C:67:VAL:HG13	1:C:68:THR:H	1.62	0.65
1:A:215:ARG:H	1:D:171:ARG:NH2	1.94	0.65
1:A:44:LEU:HD13	1:B:218:LEU:O	1.96	0.65
1:A:104:PHE:O	1:A:107:LYS:HB2	1.97	0.65
1:A:67:VAL:HG13	1:A:68:THR:H	1.62	0.65
1:A:189:LEU:HA	1:B:71:PHE:CZ	2.32	0.65
1:D:155:HIS:O	1:D:158:ALA:HB3	1.97	0.65
1:A:127:GLN:HA	1:D:240:LEU:HD21	1.79	0.64
1:B:155:HIS:O	1:B:158:ALA:HB3	1.97	0.64
1:C:104:PHE:O	1:C:107:LYS:HB2	1.97	0.64
1:B:123:ARG:O	1:B:127:GLN:HB2	1.96	0.64
1:D:123:ARG:O	1:D:127:GLN:HB2	1.97	0.64
1:D:126:LEU:HD23	1:D:127:GLN:H	1.61	0.64
1:C:189:LEU:HA	1:D:71:PHE:CZ	2.32	0.64
1:C:44:LEU:HD21	1:D:219:LEU:O	1.97	0.64
1:C:141:LEU:C	1:C:143:PRO:HD2	2.24	0.63
1:A:141:LEU:O	1:A:144:LEU:HD22	1.98	0.63
1:A:141:LEU:C	1:A:143:PRO:HD2	2.24	0.63
1:D:111:GLU:O	1:D:114:LEU:HB3	1.99	0.63
1:B:111:GLU:O	1:B:114:LEU:HB3	1.99	0.62
1:B:126:LEU:HD23	1:B:127:GLN:H	1.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:O	1:C:144:LEU:HD22	1.98	0.62
1:B:98:GLN:HA	1:B:98:GLN:NE2	2.14	0.62
1:D:44:LEU:HB3	1:D:47:LEU:HB2	1.81	0.62
1:D:144:LEU:HA	1:D:147:GLU:HB2	1.82	0.62
1:D:108:TRP:NE1	1:D:112:MET:SD	2.73	0.62
1:A:221:VAL:HG21	1:B:45:LYS:HD3	1.82	0.62
1:B:219:LEU:HB3	1:B:220:PRO:HD2	1.81	0.62
1:B:108:TRP:NE1	1:B:112:MET:SD	2.73	0.61
1:C:93:VAL:CG2	1:D:170:LEU:HD11	2.31	0.61
1:A:49:ASN:HB2	1:D:90:LEU:HD22	1.81	0.61
1:B:44:LEU:HB3	1:B:47:LEU:HB2	1.81	0.61
1:A:142:SER:N	1:A:143:PRO:CD	2.64	0.61
1:A:174:LEU:O	1:A:177:ARG:HB2	2.00	0.61
1:B:222:LEU:HD23	1:C:156:VAL:HG11	1.83	0.61
1:D:219:LEU:HB3	1:D:220:PRO:HD2	1.81	0.61
1:D:226:LYS:O	1:D:227:VAL:HG13	2.01	0.61
1:A:57:PHE:HB3	1:D:79:THR:HG23	1.82	0.61
1:A:93:VAL:HG11	1:B:170:LEU:CD2	2.31	0.61
1:C:203:LEU:HD21	1:D:60:LEU:HD13	1.83	0.61
1:B:222:LEU:HD21	1:C:156:VAL:HG11	1.83	0.60
1:C:124:ALA:HA	1:C:127:GLN:HB3	1.83	0.60
1:C:174:LEU:O	1:C:177:ARG:HB2	2.00	0.60
1:B:142:SER:N	1:B:143:PRO:HD2	2.16	0.60
1:B:144:LEU:HA	1:B:147:GLU:HB2	1.82	0.60
1:B:138:GLN:O	1:B:142:SER:HB2	2.01	0.60
1:B:226:LYS:O	1:B:227:VAL:HG13	2.01	0.60
1:D:142:SER:N	1:D:143:PRO:HD2	2.16	0.60
1:A:128:GLU:HA	1:A:131:ARG:HD2	1.82	0.60
1:C:221:VAL:HG21	1:D:45:LYS:HD3	1.82	0.60
1:A:73:ASP:O	1:A:77:LYS:HB2	2.02	0.60
1:D:138:GLN:O	1:D:142:SER:HB2	2.01	0.60
1:A:177:ARG:CZ	1:B:86:MET:HA	2.32	0.60
1:C:128:GLU:HA	1:C:131:ARG:HD2	1.82	0.60
1:C:142:SER:N	1:C:143:PRO:CD	2.64	0.60
1:A:156:VAL:HG11	1:D:222:LEU:CD2	2.32	0.60
1:A:203:LEU:HD21	1:B:60:LEU:HD13	1.83	0.60
1:A:104:PHE:CE2	1:B:155:HIS:HB3	2.37	0.60
1:B:141:LEU:C	1:B:143:PRO:HD2	2.27	0.60
1:B:198:GLU:O	1:B:202:THR:HG23	2.02	0.60
1:C:93:VAL:HG11	1:D:170:LEU:CD2	2.32	0.60
1:C:104:PHE:CE2	1:D:155:HIS:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:CZ	1:D:86:MET:HA	2.32	0.59
1:D:198:GLU:O	1:D:202:THR:HG23	2.02	0.59
1:A:93:VAL:CG2	1:B:170:LEU:HD11	2.31	0.59
1:A:59:LYS:HG3	1:A:63:GLN:HG3	1.84	0.59
1:B:171:ARG:NE	1:C:215:ARG:HB2	2.12	0.59
1:A:124:ALA:HA	1:A:127:GLN:HB3	1.83	0.59
1:B:105:GLN:OE1	1:B:105:GLN:HA	2.01	0.59
1:C:120:GLU:O	1:C:123:ARG:HB3	2.02	0.59
1:D:141:LEU:C	1:D:143:PRO:HD2	2.27	0.59
1:D:105:GLN:HA	1:D:105:GLN:OE1	2.01	0.59
1:A:120:GLU:O	1:A:123:ARG:HB3	2.02	0.59
1:A:220:PRO:C	1:A:222:LEU:H	2.10	0.59
1:B:90:LEU:HD22	1:C:49:ASN:HB2	1.84	0.59
1:D:98:GLN:HA	1:D:98:GLN:NE2	2.14	0.59
1:B:225:PHE:CB	1:C:148:MET:HE1	2.33	0.59
1:B:227:VAL:HG23	1:B:230:LEU:HB2	1.85	0.58
1:C:59:LYS:HG3	1:C:63:GLN:HG3	1.84	0.58
1:A:134:LEU:HD23	1:A:134:LEU:N	2.18	0.58
1:D:227:VAL:HG23	1:D:230:LEU:HB2	1.85	0.58
1:C:73:ASP:O	1:C:77:LYS:HB2	2.02	0.58
1:C:134:LEU:HD23	1:C:134:LEU:N	2.18	0.58
1:C:220:PRO:C	1:C:222:LEU:H	2.10	0.58
1:B:80:GLU:HG3	1:B:83:ARG:HD3	1.86	0.58
1:D:229:PHE:CD1	1:D:229:PHE:N	2.68	0.58
1:C:199:HIS:CD2	1:D:63:GLN:HB3	2.39	0.58
1:B:65:GLY:N	1:B:66:PRO:CD	2.67	0.58
1:B:95:ALA:O	1:B:99:PRO:HD2	2.04	0.58
1:C:80:GLU:HA	1:C:83:ARG:HB3	1.86	0.58
1:D:80:GLU:HG3	1:D:83:ARG:HD3	1.86	0.57
1:C:101:LEU:HG	1:C:102:ASP:N	2.19	0.57
1:A:71:PHE:CE1	1:B:189:LEU:HA	2.39	0.57
1:D:95:ALA:O	1:D:99:PRO:HD2	2.04	0.57
1:A:199:HIS:CD2	1:B:63:GLN:HB3	2.39	0.57
1:C:177:ARG:NH1	1:D:86:MET:SD	2.78	0.57
1:D:65:GLY:N	1:D:66:PRO:CD	2.67	0.57
1:A:130:ALA:O	1:A:134:LEU:HG	2.05	0.57
1:C:71:PHE:CE1	1:D:189:LEU:HA	2.39	0.57
1:C:130:ALA:O	1:C:134:LEU:HG	2.05	0.57
1:B:229:PHE:N	1:B:229:PHE:CD1	2.68	0.57
1:A:153:ARG:O	1:A:156:VAL:HB	2.05	0.57
1:D:64:LEU:O	1:D:67:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:VAL:C	1:D:121:PRO:HD2	2.30	0.56
1:A:221:VAL:CG1	1:B:45:LYS:HG2	2.35	0.56
1:B:64:LEU:O	1:B:67:VAL:HG23	2.04	0.56
1:B:119:VAL:C	1:B:121:PRO:HD2	2.30	0.56
1:A:80:GLU:HA	1:A:83:ARG:HB3	1.86	0.56
1:A:100:TYR:O	1:A:103:ASP:HB3	2.06	0.56
1:A:144:LEU:O	1:A:148:MET:HB3	2.06	0.56
1:A:177:ARG:NH1	1:B:86:MET:SD	2.78	0.56
1:B:69:GLN:O	1:B:73:ASP:HB3	2.05	0.56
1:C:153:ARG:O	1:C:156:VAL:HB	2.05	0.56
1:C:189:LEU:HA	1:D:71:PHE:CE1	2.40	0.56
1:A:101:LEU:HG	1:A:102:ASP:N	2.19	0.56
1:C:100:TYR:O	1:C:103:ASP:HB3	2.06	0.56
1:C:221:VAL:CG1	1:D:45:LYS:HG2	2.35	0.56
1:A:189:LEU:HA	1:B:71:PHE:CE1	2.40	0.56
1:D:69:GLN:O	1:D:73:ASP:HB3	2.05	0.56
1:C:227:VAL:HG11	1:C:230:LEU:CB	2.35	0.56
1:A:163:LEU:C	1:A:165:PRO:HD2	2.31	0.56
1:A:227:VAL:HG11	1:A:230:LEU:CB	2.35	0.56
1:C:64:LEU:C	1:C:66:PRO:HD2	2.31	0.55
1:D:90:LEU:O	1:D:94:LYS:HB2	2.05	0.55
1:B:227:VAL:HG23	1:B:230:LEU:N	2.19	0.55
1:B:49:ASN:HD22	1:C:94:LYS:HE3	1.67	0.55
1:B:164:ALA:N	1:B:165:PRO:HD2	2.21	0.55
1:C:65:GLY:N	1:C:66:PRO:CD	2.70	0.55
1:C:144:LEU:O	1:C:148:MET:HB3	2.06	0.55
1:A:65:GLY:N	1:A:66:PRO:CD	2.70	0.55
1:B:90:LEU:O	1:B:94:LYS:HB2	2.05	0.55
1:C:123:ARG:O	1:C:127:GLN:N	2.38	0.55
1:A:64:LEU:C	1:A:66:PRO:HD2	2.31	0.55
1:A:156:VAL:HG11	1:D:222:LEU:HD21	1.88	0.55
1:C:199:HIS:NE2	1:D:63:GLN:HB3	2.22	0.55
1:A:94:LYS:HE2	1:D:46:LEU:CB	2.37	0.55
1:C:163:LEU:C	1:C:165:PRO:HD2	2.31	0.55
1:A:90:LEU:O	1:A:93:VAL:HB	2.08	0.55
1:A:214:LEU:HD11	1:B:48:ASP:O	2.07	0.55
1:C:229:PHE:O	1:C:232:ALA:HB3	2.07	0.54
1:C:214:LEU:HD11	1:D:48:ASP:O	2.07	0.54
1:B:240:LEU:HD21	1:C:127:GLN:HA	1.89	0.54
1:A:157:ASP:O	1:A:160:ARG:HB3	2.08	0.54
1:C:71:PHE:C	1:C:75:LEU:HG	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:O	1:C:93:VAL:HB	2.08	0.54
1:C:118:LYS:O	1:C:121:PRO:HD2	2.08	0.54
1:D:66:PRO:CA	1:D:69:GLN:HB3	2.26	0.54
1:A:134:LEU:HD13	1:D:233:LEU:HB3	1.90	0.54
1:C:157:ASP:O	1:C:160:ARG:HB3	2.08	0.54
1:A:199:HIS:NE2	1:B:63:GLN:HB3	2.22	0.54
1:D:164:ALA:N	1:D:165:PRO:HD2	2.21	0.54
1:A:71:PHE:C	1:A:75:LEU:HG	2.32	0.53
1:A:123:ARG:O	1:A:127:GLN:N	2.38	0.53
1:C:192:TYR:HA	1:D:70:GLU:OE1	2.08	0.53
1:D:80:GLU:O	1:D:83:ARG:HB3	2.08	0.53
1:A:229:PHE:O	1:A:232:ALA:HB3	2.07	0.53
1:B:171:ARG:HH22	1:C:214:LEU:H	1.56	0.53
1:C:214:LEU:HD11	1:D:49:ASN:HA	1.91	0.53
1:A:192:TYR:HA	1:B:70:GLU:OE1	2.08	0.53
1:A:46:LEU:C	1:A:48:ASP:H	2.17	0.53
1:B:163:LEU:C	1:B:165:PRO:HD2	2.34	0.53
1:A:67:VAL:HA	1:B:192:TYR:CE1	2.44	0.53
1:A:71:PHE:CZ	1:B:189:LEU:HA	2.44	0.53
1:A:118:LYS:O	1:A:121:PRO:HD2	2.08	0.53
1:A:237:THR:HA	1:A:240:LEU:CG	2.39	0.53
1:C:71:PHE:CZ	1:D:189:LEU:HA	2.44	0.53
1:B:80:GLU:O	1:B:83:ARG:HB3	2.08	0.52
1:C:228:SER:O	1:C:231:SER:HB3	2.09	0.52
1:C:67:VAL:HA	1:D:192:TYR:CE1	2.44	0.52
1:A:214:LEU:HD11	1:B:49:ASN:HA	1.91	0.52
1:D:163:LEU:C	1:D:165:PRO:HD2	2.34	0.52
1:C:144:LEU:HD13	1:C:144:LEU:N	2.25	0.52
1:D:227:VAL:CG2	1:D:230:LEU:HB2	2.40	0.52
1:A:231:SER:O	1:A:234:GLU:HB2	2.10	0.52
1:B:46:LEU:CB	1:C:94:LYS:HE2	2.38	0.52
1:D:227:VAL:HG23	1:D:230:LEU:N	2.19	0.52
1:A:99:PRO:O	1:A:102:ASP:HB2	2.10	0.52
1:C:227:VAL:HG12	1:C:230:LEU:HB3	1.92	0.52
1:D:146:GLU:CA	1:D:149:ARG:HB3	2.40	0.52
1:A:144:LEU:HD13	1:A:144:LEU:N	2.25	0.52
1:A:152:ALA:O	1:A:153:ARG:C	2.53	0.51
1:B:146:GLU:CA	1:B:149:ARG:HB3	2.40	0.51
1:B:227:VAL:CG2	1:B:230:LEU:HB2	2.40	0.51
1:B:233:LEU:HB3	1:C:134:LEU:HD13	1.92	0.51
1:D:162:HIS:C	1:D:163:LEU:HD23	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:O	1:A:231:SER:HB3	2.09	0.51
1:B:174:LEU:HA	1:B:177:ARG:HB3	1.91	0.51
1:C:231:SER:O	1:C:234:GLU:HB2	2.10	0.51
1:D:174:LEU:HA	1:D:177:ARG:HB3	1.91	0.51
1:B:78:GLU:O	1:B:82:LEU:HG	2.10	0.51
1:A:198:GLU:O	1:A:202:THR:HG23	2.11	0.51
1:C:46:LEU:C	1:C:48:ASP:H	2.17	0.51
1:D:228:SER:O	1:D:232:ALA:N	2.41	0.51
1:B:48:ASP:O	1:B:51:ASP:HB2	2.11	0.51
1:C:198:GLU:O	1:C:202:THR:HG23	2.11	0.51
1:B:162:HIS:C	1:B:163:LEU:HD23	2.35	0.51
1:C:99:PRO:O	1:C:102:ASP:HB2	2.10	0.51
1:C:152:ALA:O	1:C:153:ARG:C	2.53	0.51
1:D:78:GLU:O	1:D:82:LEU:HG	2.10	0.51
1:D:235:GLU:O	1:D:238:LYS:HB3	2.11	0.50
1:B:235:GLU:O	1:B:238:LYS:HB3	2.11	0.50
1:C:67:VAL:O	1:C:71:PHE:HB2	2.10	0.50
1:C:237:THR:HA	1:C:240:LEU:CG	2.39	0.50
1:D:108:TRP:CE2	1:D:112:MET:SD	3.05	0.50
1:B:153:ARG:O	1:B:156:VAL:HB	2.11	0.50
1:D:93:VAL:O	1:D:97:VAL:HG23	2.11	0.50
1:A:48:ASP:C	1:A:50:TRP:N	2.68	0.50
1:B:123:ARG:HA	1:B:126:LEU:HD22	1.94	0.50
1:B:93:VAL:O	1:B:97:VAL:HG23	2.11	0.50
1:B:228:SER:O	1:B:232:ALA:N	2.41	0.50
1:D:93:VAL:HG23	1:D:94:LYS:N	2.27	0.50
1:A:67:VAL:O	1:A:71:PHE:HB2	2.10	0.50
1:B:79:THR:HG23	1:C:57:PHE:HB3	1.92	0.50
1:D:153:ARG:O	1:D:156:VAL:HB	2.11	0.50
1:A:169:GLU:O	1:A:173:ARG:HG3	2.10	0.50
1:C:48:ASP:C	1:C:50:TRP:N	2.68	0.50
1:C:169:GLU:O	1:C:173:ARG:HG3	2.10	0.50
1:D:123:ARG:HA	1:D:126:LEU:HD22	1.94	0.50
1:D:136:GLU:O	1:D:140:LYS:HB3	2.12	0.50
1:B:66:PRO:CA	1:B:69:GLN:HB3	2.26	0.50
1:B:108:TRP:CE2	1:B:112:MET:SD	3.05	0.50
1:D:48:ASP:O	1:D:51:ASP:HB2	2.11	0.50
1:D:66:PRO:HA	1:D:69:GLN:CB	2.29	0.50
1:A:115:TYR:C	1:A:117:GLN:N	2.70	0.49
1:B:136:GLU:O	1:B:140:LYS:CB	2.60	0.49
1:A:83:ARG:HG3	1:D:53:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:O	1:B:104:PHE:HB3	2.13	0.49
1:B:93:VAL:HG23	1:B:94:LYS:N	2.27	0.49
1:B:241:ASN:HA	1:C:123:ARG:HH21	1.77	0.49
1:C:86:MET:SD	1:D:177:ARG:HD2	2.53	0.49
1:B:136:GLU:O	1:B:140:LYS:HB3	2.12	0.49
1:A:86:MET:SD	1:B:177:ARG:HD2	2.53	0.49
1:D:136:GLU:O	1:D:140:LYS:CB	2.60	0.49
1:A:222:LEU:HD23	1:A:223:GLU:N	2.28	0.49
1:B:65:GLY:N	1:B:66:PRO:HD2	2.27	0.49
1:D:49:ASN:O	1:D:53:VAL:HG23	2.13	0.49
1:D:88:LYS:O	1:D:92:GLU:HG3	2.12	0.49
1:B:49:ASN:O	1:B:53:VAL:HG23	2.13	0.49
1:B:88:LYS:O	1:B:92:GLU:HG3	2.12	0.49
1:C:101:LEU:O	1:C:104:PHE:N	2.45	0.49
1:D:101:LEU:O	1:D:104:PHE:HB3	2.13	0.49
1:A:101:LEU:O	1:A:104:PHE:N	2.45	0.48
1:B:207:ALA:C	1:B:209:PRO:HD2	2.38	0.48
1:C:115:TYR:C	1:C:117:GLN:N	2.70	0.48
1:D:186:GLY:O	1:D:189:LEU:HB3	2.14	0.48
1:B:169:GLU:O	1:B:173:ARG:HB2	2.13	0.48
1:B:186:GLY:O	1:B:189:LEU:HB3	2.13	0.48
1:A:159:LEU:O	1:A:160:ARG:C	2.56	0.48
1:C:117:GLN:O	1:C:121:PRO:HD3	2.14	0.48
1:A:117:GLN:O	1:A:121:PRO:HD3	2.14	0.48
1:B:71:PHE:O	1:B:75:LEU:HB2	2.13	0.48
1:C:222:LEU:HD23	1:C:223:GLU:N	2.28	0.48
1:D:207:ALA:C	1:D:209:PRO:HD2	2.38	0.48
1:B:146:GLU:O	1:B:149:ARG:HB3	2.13	0.48
1:D:63:GLN:O	1:D:66:PRO:HD2	2.14	0.48
1:C:67:VAL:HG13	1:C:68:THR:N	2.27	0.48
1:D:65:GLY:N	1:D:66:PRO:HD2	2.27	0.48
1:D:146:GLU:O	1:D:149:ARG:HB3	2.13	0.48
1:D:164:ALA:HA	1:D:167:SER:HB3	1.95	0.48
1:A:144:LEU:N	1:A:144:LEU:CD1	2.77	0.48
1:A:159:LEU:HA	1:A:162:HIS:HB2	1.96	0.48
1:B:180:ALA:O	1:B:184:ASN:ND2	2.47	0.48
1:A:227:VAL:HG12	1:A:230:LEU:HB3	1.92	0.48
1:B:63:GLN:O	1:B:66:PRO:HD2	2.14	0.48
1:D:120:GLU:N	1:D:121:PRO:HD2	2.29	0.48
1:A:233:LEU:HA	1:A:236:TYR:HB3	1.96	0.47
1:D:71:PHE:O	1:D:75:LEU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLU:N	1:B:121:PRO:HD2	2.29	0.47
1:C:227:VAL:HG22	1:C:229:PHE:CZ	2.49	0.47
1:C:219:LEU:HB3	1:C:220:PRO:HD3	1.96	0.47
1:C:237:THR:HA	1:C:240:LEU:CD1	2.44	0.47
1:C:159:LEU:HA	1:C:162:HIS:HB2	1.96	0.47
1:C:233:LEU:HA	1:C:236:TYR:HB3	1.96	0.47
1:A:67:VAL:HG13	1:A:68:THR:N	2.27	0.47
1:B:164:ALA:HA	1:B:167:SER:HB3	1.95	0.47
1:C:159:LEU:O	1:C:160:ARG:C	2.56	0.47
1:A:237:THR:HA	1:A:240:LEU:CD1	2.44	0.47
1:A:239:LYS:HA	1:A:242:THR:OG1	2.15	0.47
1:C:44:LEU:HD11	1:D:219:LEU:O	2.15	0.47
1:C:63:GLN:HB3	1:D:199:HIS:NE2	2.30	0.47
1:C:188:ARG:HG3	1:D:74:ASN:HD22	1.80	0.47
1:D:169:GLU:O	1:D:173:ARG:HB2	2.13	0.47
1:A:220:PRO:C	1:A:222:LEU:N	2.73	0.47
1:B:165:PRO:HG2	1:B:166:TYR:CD2	2.50	0.47
1:C:144:LEU:N	1:C:144:LEU:CD1	2.77	0.47
1:A:227:VAL:HG22	1:A:229:PHE:CZ	2.49	0.47
1:B:46:LEU:O	1:B:49:ASN:CG	2.58	0.47
1:C:65:GLY:C	1:C:67:VAL:H	2.23	0.47
1:A:188:ARG:HG3	1:B:74:ASN:HD22	1.80	0.46
1:C:239:LYS:HA	1:C:242:THR:OG1	2.15	0.46
1:D:46:LEU:O	1:D:49:ASN:CG	2.58	0.46
1:A:44:LEU:HD11	1:B:219:LEU:O	2.15	0.46
1:A:215:ARG:HB2	1:D:171:ARG:NE	2.23	0.46
1:C:144:LEU:HD23	1:D:115:TYR:OH	2.15	0.46
1:D:91:GLU:O	1:D:94:LYS:HB3	2.16	0.46
1:A:63:GLN:HB3	1:B:199:HIS:NE2	2.30	0.46
1:A:123:ARG:HH21	1:D:241:ASN:HA	1.79	0.46
1:B:49:ASN:HD21	1:C:94:LYS:HE3	1.77	0.46
1:B:208:LYS:HA	1:B:211:LEU:CD1	2.42	0.46
1:C:220:PRO:C	1:C:222:LEU:N	2.73	0.46
1:D:227:VAL:HG23	1:D:230:LEU:CB	2.45	0.46
1:B:91:GLU:O	1:B:94:LYS:HB3	2.16	0.46
1:B:219:LEU:CB	1:B:220:PRO:HD2	2.44	0.46
1:D:180:ALA:O	1:D:184:ASN:ND2	2.47	0.46
1:D:165:PRO:HG2	1:D:166:TYR:CD2	2.50	0.46
1:B:93:VAL:CG2	1:B:94:LYS:N	2.79	0.46
1:A:48:ASP:O	1:A:51:ASP:N	2.49	0.46
1:A:94:LYS:HE3	1:D:49:ASN:HD22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:NZ	1:D:44:LEU:HD22	2.30	0.46
1:A:94:LYS:CE	1:D:46:LEU:HB2	2.42	0.46
1:A:144:LEU:HD23	1:B:115:TYR:OH	2.15	0.46
1:B:60:LEU:O	1:B:63:GLN:HB2	2.16	0.46
1:B:156:VAL:C	1:B:158:ALA:N	2.73	0.46
1:B:218:LEU:HD23	1:C:167:SER:OG	2.16	0.46
1:D:93:VAL:CG2	1:D:94:LYS:N	2.79	0.46
1:A:115:TYR:CD1	1:B:148:MET:SD	3.09	0.46
1:C:48:ASP:O	1:C:51:ASP:N	2.49	0.46
1:D:107:LYS:O	1:D:110:GLU:HB2	2.15	0.46
1:D:159:LEU:HD21	1:D:163:LEU:HD11	1.98	0.46
1:A:211:LEU:O	1:D:171:ARG:NE	2.50	0.45
1:B:171:ARG:NE	1:C:211:LEU:O	2.49	0.45
1:C:97:VAL:O	1:C:98:GLN:C	2.59	0.45
1:C:229:PHE:CD1	1:C:229:PHE:N	2.82	0.45
1:D:230:LEU:HD12	1:D:230:LEU:HA	1.58	0.45
1:A:189:LEU:HA	1:B:71:PHE:HZ	1.81	0.45
1:A:233:LEU:HD22	1:A:233:LEU:N	2.32	0.45
1:C:167:SER:O	1:C:171:ARG:HG3	2.15	0.45
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.67	0.45
1:A:65:GLY:C	1:A:67:VAL:H	2.23	0.45
1:B:174:LEU:C	1:B:174:LEU:HD12	2.41	0.45
1:D:219:LEU:CB	1:D:220:PRO:HD2	2.44	0.45
1:A:97:VAL:O	1:A:98:GLN:C	2.59	0.45
1:D:53:VAL:O	1:D:57:PHE:HD2	1.99	0.45
1:A:85:GLU:O	1:A:89:ASP:HB2	2.17	0.45
1:A:219:LEU:HB3	1:A:220:PRO:HD3	1.96	0.45
1:B:135:HIS:HA	1:B:138:GLN:HB3	1.98	0.45
1:B:225:PHE:HB2	1:C:148:MET:HE1	1.96	0.45
1:D:174:LEU:C	1:D:174:LEU:HD12	2.41	0.45
1:A:48:ASP:C	1:A:50:TRP:H	2.25	0.45
1:A:57:PHE:HB3	1:D:79:THR:CG2	2.44	0.45
1:B:123:ARG:O	1:B:126:LEU:HD23	2.17	0.45
1:B:167:SER:O	1:B:171:ARG:HG2	2.17	0.45
1:C:115:TYR:CD1	1:D:148:MET:SD	3.10	0.45
1:D:156:VAL:C	1:D:158:ALA:N	2.73	0.45
1:A:167:SER:O	1:A:171:ARG:HG3	2.15	0.45
1:B:146:GLU:HA	1:B:149:ARG:CB	2.45	0.45
1:A:227:VAL:HG13	1:A:229:PHE:CZ	2.52	0.45
1:A:229:PHE:CD1	1:A:229:PHE:N	2.82	0.45
1:C:85:GLU:O	1:C:89:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:O	1:C:102:ASP:C	2.60	0.45
1:C:152:ALA:O	1:C:156:VAL:HG23	2.17	0.45
1:B:53:VAL:O	1:B:57:PHE:HD2	1.99	0.45
1:B:171:ARG:NH2	1:C:214:LEU:N	2.65	0.45
1:C:48:ASP:C	1:C:50:TRP:H	2.25	0.45
1:D:167:SER:O	1:D:171:ARG:HG2	2.17	0.45
1:B:227:VAL:HG23	1:B:230:LEU:CB	2.45	0.44
1:D:60:LEU:O	1:D:63:GLN:HB2	2.16	0.44
1:C:102:ASP:O	1:C:103:ASP:C	2.61	0.44
1:C:233:LEU:N	1:C:233:LEU:HD22	2.32	0.44
1:D:135:HIS:HA	1:D:138:GLN:HB3	1.98	0.44
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.66	0.44
1:B:159:LEU:HD21	1:B:163:LEU:HD11	1.99	0.44
1:C:157:ASP:O	1:C:158:ALA:C	2.60	0.44
1:B:107:LYS:O	1:B:110:GLU:HB2	2.15	0.44
1:A:60:LEU:O	1:A:64:LEU:HB2	2.18	0.44
1:A:156:VAL:HG11	1:D:222:LEU:HD23	1.98	0.44
1:B:155:HIS:ND1	1:B:155:HIS:N	2.65	0.44
1:C:170:LEU:HA	1:C:170:LEU:HD23	1.65	0.44
1:A:219:LEU:HB3	1:A:220:PRO:CD	2.48	0.44
1:C:164:ALA:N	1:C:165:PRO:HD2	2.33	0.44
1:A:70:GLU:O	1:A:74:ASN:HB2	2.18	0.44
1:B:109:GLN:HA	1:B:109:GLN:OE1	2.18	0.44
1:C:70:GLU:O	1:C:74:ASN:HB2	2.18	0.44
1:C:219:LEU:HB3	1:C:220:PRO:CD	2.48	0.44
1:D:123:ARG:O	1:D:126:LEU:HD23	2.17	0.44
1:A:152:ALA:O	1:A:156:VAL:HG23	2.17	0.43
1:A:226:LYS:O	1:A:227:VAL:C	2.61	0.43
1:C:226:LYS:O	1:C:227:VAL:C	2.61	0.43
1:A:164:ALA:N	1:A:165:PRO:HD2	2.33	0.43
1:C:59:LYS:O	1:C:63:GLN:HB2	2.18	0.43
1:D:109:GLN:HA	1:D:109:GLN:OE1	2.18	0.43
1:A:101:LEU:O	1:A:102:ASP:C	2.60	0.43
1:A:59:LYS:O	1:A:63:GLN:HB2	2.18	0.43
1:A:114:LEU:O	1:A:117:GLN:HB2	2.18	0.43
1:A:122:LEU:N	1:A:122:LEU:HD23	2.33	0.43
1:C:174:LEU:HD13	1:D:86:MET:SD	2.59	0.43
1:A:67:VAL:HB	1:B:192:TYR:OH	2.19	0.43
1:A:211:LEU:O	1:D:171:ARG:CZ	2.67	0.43
1:A:225:PHE:HZ	1:C:115:TYR:CE2	2.36	0.43
1:D:86:MET:SD	1:D:86:MET:C	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:VAL:HG13	1:C:229:PHE:CZ	2.52	0.43
1:D:233:LEU:HA	1:D:233:LEU:HD23	1.74	0.43
1:C:114:LEU:O	1:C:117:GLN:HB2	2.18	0.43
1:A:113:GLU:O	1:A:117:GLN:HG2	2.18	0.43
1:A:157:ASP:O	1:A:158:ALA:C	2.60	0.43
1:B:203:LEU:C	1:B:205:GLU:H	2.26	0.43
1:D:203:LEU:C	1:D:205:GLU:H	2.26	0.43
1:D:208:LYS:HA	1:D:211:LEU:CD1	2.42	0.43
1:A:94:LYS:HZ3	1:D:44:LEU:HD22	1.83	0.43
1:A:200:LEU:N	1:A:200:LEU:HD23	2.34	0.43
1:C:113:GLU:O	1:C:117:GLN:HG2	2.18	0.43
1:C:159:LEU:O	1:C:163:LEU:N	2.51	0.43
1:D:89:ASP:HA	1:D:92:GLU:OE2	2.19	0.43
1:A:102:ASP:O	1:A:103:ASP:C	2.61	0.42
1:A:159:LEU:O	1:A:163:LEU:N	2.51	0.42
1:A:174:LEU:HD13	1:B:86:MET:SD	2.59	0.42
1:C:122:LEU:N	1:C:122:LEU:HD23	2.33	0.42
1:D:148:MET:O	1:D:149:ARG:C	2.62	0.42
1:A:167:SER:OG	1:D:218:LEU:HD23	2.18	0.42
1:C:115:TYR:C	1:C:117:GLN:H	2.27	0.42
1:C:60:LEU:O	1:C:64:LEU:HB2	2.18	0.42
1:C:177:ARG:NH2	1:D:85:GLU:O	2.52	0.42
1:A:49:ASN:HD21	1:D:87:SER:HA	1.84	0.42
1:A:127:GLN:HG3	1:D:240:LEU:HD21	2.01	0.42
1:A:148:MET:HE1	1:D:225:PHE:CB	2.49	0.42
1:B:146:GLU:O	1:B:147:GLU:C	2.62	0.42
1:C:200:LEU:N	1:C:200:LEU:HD23	2.34	0.42
1:D:229:PHE:O	1:D:232:ALA:HB3	2.20	0.42
1:A:177:ARG:NH2	1:B:85:GLU:O	2.52	0.42
1:C:67:VAL:HB	1:D:192:TYR:OH	2.19	0.42
1:A:119:VAL:O	1:A:122:LEU:HG	2.20	0.42
1:C:65:GLY:C	1:C:67:VAL:N	2.78	0.42
1:D:47:LEU:C	1:D:49:ASN:H	2.28	0.42
1:A:65:GLY:C	1:A:67:VAL:N	2.78	0.42
1:B:86:MET:SD	1:B:86:MET:C	3.01	0.42
1:C:119:VAL:O	1:C:122:LEU:HG	2.20	0.42
1:A:217:GLY:O	1:A:221:VAL:HG22	2.20	0.42
1:B:47:LEU:C	1:B:49:ASN:H	2.28	0.42
1:D:146:GLU:O	1:D:147:GLU:C	2.62	0.42
1:C:98:GLN:OE1	1:C:102:ASP:CG	2.63	0.41
1:D:120:GLU:HA	1:D:123:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HG	1:A:122:LEU:H	1.58	0.41
1:A:144:LEU:HD13	1:A:144:LEU:H	1.85	0.41
1:B:89:ASP:HA	1:B:92:GLU:OE2	2.19	0.41
1:B:215:ARG:O	1:B:218:LEU:HB2	2.20	0.41
1:B:229:PHE:O	1:B:232:ALA:HB3	2.20	0.41
1:D:95:ALA:O	1:D:99:PRO:CD	2.68	0.41
1:A:98:GLN:OE1	1:A:102:ASP:CG	2.63	0.41
1:B:233:LEU:HA	1:B:233:LEU:HD23	1.74	0.41
1:B:240:LEU:HD21	1:C:127:GLN:HG3	2.02	0.41
1:C:47:LEU:C	1:C:49:ASN:H	2.28	0.41
1:A:222:LEU:HD23	1:A:223:GLU:H	1.86	0.41
1:B:46:LEU:HB2	1:C:94:LYS:CE	2.47	0.41
1:B:148:MET:O	1:B:149:ARG:C	2.62	0.41
1:C:144:LEU:HD13	1:C:144:LEU:H	1.85	0.41
1:C:222:LEU:HD23	1:C:223:GLU:H	1.86	0.41
1:A:47:LEU:C	1:A:49:ASN:H	2.28	0.41
1:B:120:GLU:HA	1:B:123:ARG:HG3	2.01	0.41
1:C:44:LEU:HG	1:D:221:VAL:HG23	2.02	0.41
1:C:233:LEU:HA	1:C:233:LEU:HD13	1.83	0.41
1:A:115:TYR:C	1:A:117:GLN:H	2.27	0.41
1:C:144:LEU:HB3	1:D:115:TYR:CE2	2.56	0.41
1:B:109:GLN:O	1:B:110:GLU:C	2.64	0.41
1:C:217:GLY:O	1:C:221:VAL:HG22	2.20	0.41
1:C:48:ASP:O	1:C:50:TRP:N	2.54	0.41
1:D:210:ALA:O	1:D:214:LEU:N	2.53	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.90	0.41
1:B:93:VAL:O	1:B:94:LYS:C	2.63	0.41
1:D:93:VAL:O	1:D:94:LYS:C	2.63	0.41
1:D:211:LEU:HB2	1:D:212:GLU:OE2	2.21	0.41
1:D:214:LEU:O	1:D:215:ARG:C	2.64	0.41
1:D:215:ARG:O	1:D:218:LEU:HB2	2.20	0.41
1:A:48:ASP:O	1:A:50:TRP:N	2.54	0.41
1:A:57:PHE:CE2	1:D:83:ARG:HA	2.55	0.41
1:A:227:VAL:HG12	1:A:228:SER:N	2.36	0.41
1:A:227:VAL:HG13	1:A:229:PHE:CE1	2.56	0.41
1:B:81:GLY:O	1:B:84:GLN:HB3	2.21	0.41
1:D:174:LEU:O	1:D:178:LEU:N	2.54	0.40
1:D:203:LEU:C	1:D:205:GLU:N	2.79	0.40
1:A:144:LEU:HB3	1:B:115:TYR:CE2	2.56	0.40
1:A:166:TYR:O	1:A:167:SER:C	2.65	0.40
1:B:53:VAL:CG1	1:C:83:ARG:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:HB2	1:C:171:ARG:HH21	1.87	0.40
1:A:44:LEU:HG	1:B:221:VAL:HG23	2.02	0.40
1:B:123:ARG:O	1:B:127:GLN:CB	2.68	0.40
1:B:174:LEU:O	1:B:178:LEU:N	2.54	0.40
1:C:189:LEU:HA	1:D:71:PHE:HZ	1.81	0.40
1:D:81:GLY:O	1:D:84:GLN:HB3	2.21	0.40
1:C:227:VAL:HG13	1:C:229:PHE:CE1	2.56	0.40
1:D:78:GLU:O	1:D:79:THR:C	2.64	0.40
1:D:163:LEU:O	1:D:164:ALA:C	2.65	0.40
1:A:63:GLN:HB3	1:B:199:HIS:HE2	1.86	0.40
1:A:221:VAL:O	1:A:223:GLU:HG3	2.22	0.40
1:B:171:ARG:CZ	1:C:211:LEU:O	2.69	0.40
1:B:214:LEU:O	1:B:215:ARG:C	2.64	0.40
1:C:227:VAL:HG12	1:C:228:SER:N	2.36	0.40
1:D:148:MET:C	1:D:150:ASP:N	2.79	0.40

All (40) 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:149:ARG:NH2	1:D:150:ASP:C[4_555]	0.52	1.68
1:B:143:PRO:CB	1:C:160:ARG:NH1[3_645]	0.99	1.21
1:A:149:ARG:CZ	1:D:150:ASP:O[4_555]	1.01	1.19
1:B:151:ARG:CA	1:C:149:ARG:NH1[3_645]	1.09	1.11
1:A:149:ARG:NH2	1:D:150:ASP:O[4_555]	1.14	1.06
1:D:150:ASP:OD1	1:D:222:LEU:CD1[4_455]	1.18	1.02
1:A:149:ARG:NH2	1:D:151:ARG:N[4_555]	1.27	0.93
1:B:143:PRO:CD	1:C:160:ARG:NH2[3_645]	1.31	0.89
1:B:143:PRO:CB	1:C:160:ARG:CZ[3_645]	1.31	0.89
1:B:143:PRO:CG	1:C:160:ARG:NH2[3_645]	1.34	0.86
1:B:158:ALA:CA	1:C:138:GLN:NE2[3_645]	1.38	0.82
1:A:149:ARG:CZ	1:D:150:ASP:C[4_555]	1.49	0.71
1:B:147:GLU:O	1:C:149:ARG:NH2[3_645]	1.50	0.70
1:B:151:ARG:CG	1:C:149:ARG:CZ[3_645]	1.70	0.50
1:A:149:ARG:NH1	1:D:150:ASP:O[4_555]	1.72	0.48
1:B:143:PRO:CG	1:C:160:ARG:CZ[3_645]	1.79	0.41
1:B:151:ARG:CB	1:C:149:ARG:NH1[3_645]	1.84	0.36
1:B:151:ARG:N	1:C:149:ARG:NH2[3_645]	1.84	0.36
1:A:138:GLN:NE2	1:D:158:ALA:O[4_555]	1.85	0.35
1:B:143:PRO:CG	1:C:160:ARG:NH1[3_645]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:CZ	1:D:151:ARG:N[4_555]	1.89	0.31
1:A:149:ARG:NH2	1:D:150:ASP:CA[4_555]	1.89	0.31
1:B:158:ALA:C	1:C:138:GLN:NE2[3_645]	1.91	0.29
1:B:143:PRO:CB	1:C:160:ARG:NH2[3_645]	1.92	0.28
1:B:151:ARG:CA	1:C:149:ARG:CZ[3_645]	1.92	0.28
1:A:149:ARG:CZ	1:D:151:ARG:CA[4_555]	1.97	0.23
1:A:149:ARG:NH1	1:D:151:ARG:C[4_555]	1.97	0.23
1:A:149:ARG:NE	1:D:150:ASP:O[4_555]	2.04	0.16
1:A:149:ARG:NH1	1:D:151:ARG:O[4_555]	2.06	0.14
1:B:151:ARG:CB	1:C:149:ARG:CZ[3_645]	2.07	0.13
1:D:150:ASP:CG	1:D:222:LEU:CD1[4_455]	2.09	0.11
1:B:151:ARG:N	1:C:149:ARG:NH1[3_645]	2.11	0.09
1:B:151:ARG:CG	1:C:149:ARG:NE[3_645]	2.13	0.07
1:B:161:THR:OG1	1:B:234:GLU:OE2[3_645]	2.13	0.07
1:B:162:HIS:NE2	1:C:135:HIS:ND1[3_645]	2.13	0.07
1:B:158:ALA:O	1:C:138:GLN:NE2[3_645]	2.14	0.06
1:B:151:ARG:CG	1:C:149:ARG:NH1[3_645]	2.18	0.02
1:B:151:ARG:CG	1:C:149:ARG:NH2[3_645]	2.18	0.02
1:B:162:HIS:CD2	1:C:135:HIS:ND1[3_645]	2.18	0.02
1:A:149:ARG:NH2	1:D:151:ARG:CA[4_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	199/201 (99%)	150 (75%)	38 (19%)	11 (6%)	 1 	 18 
1	B	199/201 (99%)	153 (77%)	46 (23%)	0	 100 	 100 
1	C	199/201 (99%)	150 (75%)	38 (19%)	11 (6%)	 1 	 18 
1	D	199/201 (99%)	153 (77%)	46 (23%)	0	 100 	 100 
All	All	796/804 (99%)	606 (76%)	168 (21%)	22 (3%)	 4 	 27 

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	228	SER
1	C	153	ARG
1	C	228	SER
1	A	225	PHE
1	C	225	PHE
1	A	79	THR
1	C	79	THR
1	A	47	LEU
1	A	236	TYR
1	C	47	LEU
1	C	236	TYR
1	A	147	GLU
1	A	164	ALA
1	A	219	LEU
1	A	227	VAL
1	C	147	GLU
1	C	164	ALA
1	C	219	LEU
1	C	227	VAL
1	A	213	ASP
1	C	213	ASP

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	177/177 (100%)	158 (89%)	19 (11%)	6	24
1	B	177/177 (100%)	151 (85%)	26 (15%)	3	16
1	C	177/177 (100%)	158 (89%)	19 (11%)	6	24
1	D	177/177 (100%)	151 (85%)	26 (15%)	3	16
All	All	708/708 (100%)	618 (87%)	90 (13%)	4	20

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	PHE
1	A	72	TRP
1	A	73	ASP
1	A	90	LEU
1	A	101	LEU
1	A	102	ASP
1	A	134	LEU
1	A	135	HIS
1	A	139	GLU
1	A	144	LEU
1	A	150	ASP
1	A	162	HIS
1	A	172	GLN
1	A	179	GLU
1	A	199	HIS
1	A	208	LYS
1	A	219	LEU
1	A	227	VAL
1	A	243	GLN
1	B	48	ASP
1	B	61	ARG
1	B	66	PRO
1	B	71	PHE
1	B	75	LEU
1	B	86	MET
1	B	98	GLN
1	B	114	LEU
1	B	126	LEU
1	B	128	GLU
1	B	141	LEU
1	B	142	SER
1	B	147	GLU
1	B	155	HIS
1	B	161	THR
1	B	162	HIS
1	B	168	ASP
1	B	170	LEU
1	B	174	LEU
1	B	189	LEU
1	B	193	HIS
1	B	218	LEU
1	B	227	VAL
1	B	229	PHE

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Mol	Chain	Res	Type
1	B	237	THR
1	B	240	LEU
1	C	71	PHE
1	C	72	TRP
1	C	73	ASP
1	C	90	LEU
1	C	101	LEU
1	C	102	ASP
1	C	134	LEU
1	C	135	HIS
1	C	139	GLU
1	C	144	LEU
1	C	150	ASP
1	C	162	HIS
1	C	172	GLN
1	C	179	GLU
1	C	199	HIS
1	C	208	LYS
1	C	219	LEU
1	C	227	VAL
1	C	243	GLN
1	D	48	ASP
1	D	61	ARG
1	D	66	PRO
1	D	71	PHE
1	D	75	LEU
1	D	86	MET
1	D	98	GLN
1	D	114	LEU
1	D	126	LEU
1	D	128	GLU
1	D	141	LEU
1	D	142	SER
1	D	147	GLU
1	D	155	HIS
1	D	161	THR
1	D	162	HIS
1	D	168	ASP
1	D	170	LEU
1	D	174	LEU
1	D	189	LEU
1	D	193	HIS

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Mol	Chain	Res	Type
1	D	218	LEU
1	D	227	VAL
1	D	229	PHE
1	D	237	THR
1	D	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	155	HIS
1	A	162	HIS
1	B	98	GLN
1	C	49	ASN
1	C	155	HIS
1	C	162	HIS
1	D	49	ASN
1	D	98	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	201/201 (100%)	2.51	129 (64%) 0 1	72, 133, 185, 200	0
1	B	201/201 (100%)	2.34	115 (57%) 0 1	64, 105, 190, 200	0
1	C	201/201 (100%)	2.54	132 (65%) 0 1	72, 133, 185, 200	0
1	D	201/201 (100%)	2.33	115 (57%) 0 1	64, 105, 190, 200	0
All	All	804/804 (100%)	2.43	491 (61%) 0 1	64, 105, 190, 200	0

All (491) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	LEU	7.5
1	C	243	GLN	7.3
1	B	55	SER	6.8
1	A	237	THR	6.7
1	B	50	TRP	6.3
1	D	51	ASP	6.1
1	B	235	GLU	6.0
1	A	84	GLN	6.0
1	A	242	THR	5.9
1	A	55	SER	5.9
1	A	213	ASP	5.9
1	C	208	LYS	5.9
1	D	136	GLU	5.8
1	D	106	LYS	5.6
1	C	235	GLU	5.6
1	D	228	SER	5.5
1	A	49	ASN	5.4
1	C	49	ASN	5.3
1	A	77	LYS	5.3
1	B	139	GLU	5.3
1	D	137	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	234	GLU	5.1
1	A	243	GLN	5.1
1	D	50	TRP	5.1
1	B	51	ASP	5.1
1	D	54	THR	5.0
1	B	52	SER	5.0
1	D	62	GLU	4.9
1	A	62	GLU	4.9
1	C	213	ASP	4.9
1	D	43	MET	4.8
1	A	219	LEU	4.8
1	C	56	THR	4.7
1	B	77	LYS	4.7
1	C	226	LYS	4.6
1	C	51	ASP	4.6
1	B	54	THR	4.6
1	D	61	ARG	4.6
1	B	243	GLN	4.6
1	A	224	SER	4.5
1	A	46	LEU	4.5
1	A	125	GLU	4.4
1	C	220	PRO	4.4
1	D	129	GLY	4.4
1	D	220	PRO	4.4
1	A	81	GLY	4.4
1	B	60	LEU	4.4
1	B	128	GLU	4.4
1	A	240	LEU	4.4
1	A	209	PRO	4.3
1	A	47	LEU	4.3
1	B	224	SER	4.3
1	C	224	SER	4.3
1	C	117	GLN	4.3
1	C	115	TYR	4.2
1	A	138	GLN	4.2
1	C	48	ASP	4.2
1	A	215	ARG	4.2
1	B	56	THR	4.2
1	B	68	THR	4.2
1	C	54	THR	4.2
1	D	79	THR	4.2
1	D	128	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	55	SER	4.2
1	C	52	SER	4.2
1	D	55	SER	4.1
1	D	57	PHE	4.1
1	A	110	GLU	4.1
1	D	45	LYS	4.1
1	A	76	GLU	4.1
1	A	54	THR	4.1
1	D	58	SER	4.1
1	D	67	VAL	4.1
1	C	43	MET	4.1
1	C	242	THR	4.1
1	D	63	GLN	4.0
1	D	74	ASN	4.0
1	B	221	VAL	4.0
1	A	108	TRP	3.9
1	A	99	PRO	3.9
1	C	132	GLN	3.9
1	C	83	ARG	3.9
1	D	49	ASN	3.9
1	C	204	SER	3.9
1	A	223	GLU	3.9
1	B	79	THR	3.9
1	C	61	ARG	3.9
1	A	80	GLU	3.9
1	B	204	SER	3.9
1	A	88	LYS	3.8
1	C	124	ALA	3.8
1	B	220	PRO	3.8
1	D	47	LEU	3.8
1	B	226	LYS	3.8
1	B	162	HIS	3.8
1	C	210	ALA	3.8
1	C	238	LYS	3.8
1	C	80	GLU	3.8
1	B	87	SER	3.8
1	C	65	GLY	3.8
1	C	50	TRP	3.8
1	D	227	VAL	3.8
1	A	73	ASP	3.8
1	A	203	LEU	3.8
1	C	215	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	216	GLN	3.7
1	A	202	THR	3.7
1	C	218	LEU	3.7
1	A	233	LEU	3.7
1	D	194	ALA	3.7
1	A	105	GLN	3.7
1	D	127	GLN	3.7
1	B	242	THR	3.7
1	B	140	LYS	3.7
1	C	229	PHE	3.6
1	B	74	ASN	3.6
1	C	231	SER	3.6
1	D	148	MET	3.6
1	B	241	ASN	3.6
1	D	192	TYR	3.6
1	A	227	VAL	3.6
1	C	68	THR	3.6
1	B	43	MET	3.6
1	C	168	ASP	3.6
1	C	214	LEU	3.6
1	C	70	GLU	3.6
1	A	79	THR	3.5
1	C	76	GLU	3.5
1	B	63	GLN	3.5
1	B	216	GLN	3.5
1	C	57	PHE	3.5
1	B	107	LYS	3.5
1	A	72	TRP	3.5
1	D	208	LYS	3.5
1	B	198	GLU	3.5
1	C	58	SER	3.5
1	A	172	GLN	3.5
1	C	239	LYS	3.5
1	B	223	GLU	3.5
1	D	167	SER	3.5
1	B	47	LEU	3.5
1	D	235	GLU	3.5
1	D	224	SER	3.5
1	C	108	TRP	3.4
1	C	59	LYS	3.4
1	D	100	TYR	3.4
1	C	138	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	52	SER	3.4
1	A	114	LEU	3.4
1	D	195	LYS	3.4
1	B	117	GLN	3.4
1	D	44	LEU	3.4
1	D	123	ARG	3.4
1	A	61	ARG	3.4
1	B	44	LEU	3.4
1	A	78	GLU	3.4
1	A	204	SER	3.4
1	B	222	LEU	3.4
1	B	61	ARG	3.4
1	D	168	ASP	3.4
1	A	74	ASN	3.3
1	D	221	VAL	3.3
1	A	218	LEU	3.3
1	C	217	GLY	3.3
1	A	50	TRP	3.3
1	A	238	LYS	3.3
1	B	58	SER	3.3
1	C	79	THR	3.3
1	B	169	GLU	3.3
1	C	62	GLU	3.3
1	C	209	PRO	3.3
1	B	195	LYS	3.3
1	D	133	LYS	3.3
1	A	115	TYR	3.3
1	A	230	LEU	3.3
1	C	60	LEU	3.3
1	D	193	HIS	3.2
1	D	78	GLU	3.2
1	B	82	LEU	3.2
1	C	47	LEU	3.2
1	A	87	SER	3.2
1	D	56	THR	3.2
1	B	69	GLN	3.2
1	A	191	GLU	3.2
1	C	72	TRP	3.2
1	C	119	VAL	3.2
1	B	150	ASP	3.2
1	C	188	ARG	3.2
1	B	136	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	241	ASN	3.2
1	B	45	LYS	3.2
1	D	188	ARG	3.2
1	D	139	GLU	3.2
1	A	231	SER	3.1
1	D	84	GLN	3.1
1	B	165	PRO	3.1
1	A	188	ARG	3.1
1	B	83	ARG	3.1
1	A	193	HIS	3.1
1	A	128	GLU	3.1
1	D	212	GLU	3.1
1	A	222	LEU	3.1
1	A	225	PHE	3.1
1	D	225	PHE	3.1
1	B	115	TYR	3.1
1	C	116	ARG	3.1
1	C	86	MET	3.1
1	A	118	LYS	3.1
1	C	122	LEU	3.1
1	C	223	GLU	3.1
1	C	66	PRO	3.1
1	D	102	ASP	3.1
1	A	207	ALA	3.1
1	B	233	LEU	3.1
1	A	239	LYS	3.1
1	B	234	GLU	3.1
1	A	129	GLY	3.0
1	A	216	GLN	3.0
1	A	220	PRO	3.0
1	C	127	GLN	3.0
1	C	185	GLY	3.0
1	C	237	THR	3.0
1	C	232	ALA	3.0
1	C	118	LYS	3.0
1	B	112	MET	3.0
1	A	195	LYS	3.0
1	A	144	LEU	3.0
1	A	170	LEU	3.0
1	B	71	PHE	3.0
1	A	183	GLU	3.0
1	B	180	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	57	PHE	3.0
1	A	167	SER	3.0
1	D	59	LYS	3.0
1	A	43	MET	3.0
1	C	85	GLU	3.0
1	D	91	GLU	3.0
1	A	45	LYS	3.0
1	C	69	GLN	3.0
1	C	197	THR	3.0
1	D	183	GLU	3.0
1	A	75	LEU	2.9
1	D	68	THR	2.9
1	B	72	TRP	2.9
1	B	202	THR	2.9
1	D	237	THR	2.9
1	B	176	ALA	2.9
1	C	207	ALA	2.9
1	B	76	GLU	2.9
1	C	139	GLU	2.9
1	B	116	ARG	2.9
1	C	189	LEU	2.9
1	C	113	GLU	2.9
1	C	146	GLU	2.9
1	B	238	LYS	2.9
1	D	60	LEU	2.9
1	A	236	TYR	2.8
1	C	227	VAL	2.8
1	C	225	PHE	2.8
1	C	135	HIS	2.8
1	B	65	GLY	2.8
1	C	63	GLN	2.8
1	A	241	ASN	2.8
1	B	239	LYS	2.8
1	D	116	ARG	2.8
1	A	208	LYS	2.8
1	C	82	LEU	2.8
1	A	142	SER	2.8
1	B	132	GLN	2.8
1	B	138	GLN	2.8
1	C	100	TYR	2.8
1	B	171	ARG	2.7
1	D	53	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	206	LYS	2.7
1	D	134	LEU	2.7
1	C	230	LEU	2.7
1	A	212	GLU	2.7
1	B	240	LEU	2.7
1	C	240	LEU	2.7
1	D	72	TRP	2.7
1	B	205	GLU	2.7
1	D	142	SER	2.7
1	D	204	SER	2.7
1	A	226	LYS	2.7
1	A	190	ALA	2.7
1	D	71	PHE	2.7
1	A	69	GLN	2.7
1	D	80	GLU	2.7
1	A	44	LEU	2.7
1	B	135	HIS	2.7
1	D	243	GLN	2.7
1	B	218	LEU	2.7
1	D	140	LYS	2.7
1	D	205	GLU	2.7
1	B	228	SER	2.7
1	D	48	ASP	2.6
1	B	230	LEU	2.6
1	C	128	GLU	2.6
1	A	59	LYS	2.6
1	C	73	ASP	2.6
1	C	71	PHE	2.6
1	B	59	LYS	2.6
1	C	202	THR	2.6
1	A	173	ARG	2.6
1	C	120	GLU	2.6
1	C	186	GLY	2.6
1	D	77	LYS	2.6
1	C	236	TYR	2.6
1	A	205	GLU	2.6
1	B	111	GLU	2.6
1	C	191	GLU	2.6
1	B	142	SER	2.6
1	A	48	ASP	2.6
1	A	67	VAL	2.6
1	B	227	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	PHE	2.5
1	A	211	LEU	2.5
1	C	145	GLY	2.5
1	B	80	GLU	2.5
1	B	131	ARG	2.5
1	D	147	GLU	2.5
1	D	87	SER	2.5
1	D	189	LEU	2.5
1	B	53	VAL	2.5
1	B	120	GLU	2.5
1	B	121	PRO	2.5
1	D	64	LEU	2.5
1	B	48	ASP	2.5
1	B	62	GLU	2.5
1	D	169	GLU	2.5
1	B	67	VAL	2.5
1	D	108	TRP	2.5
1	D	231	SER	2.5
1	A	169	GLU	2.5
1	D	191	GLU	2.5
1	C	89	ASP	2.5
1	B	75	LEU	2.5
1	C	64	LEU	2.5
1	C	81	GLY	2.5
1	A	58	SER	2.5
1	A	235	GLU	2.5
1	B	78	GLU	2.5
1	C	212	GLU	2.5
1	D	226	LYS	2.5
1	D	90	LEU	2.5
1	C	67	VAL	2.5
1	A	86	MET	2.5
1	C	199	HIS	2.5
1	D	164	ALA	2.5
1	A	234	GLU	2.5
1	B	70	GLU	2.5
1	C	222	LEU	2.5
1	D	125	GLU	2.5
1	B	155	HIS	2.5
1	A	166	TYR	2.4
1	B	188	ARG	2.4
1	B	207	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	182	LYS	2.4
1	C	46	LEU	2.4
1	D	236	TYR	2.4
1	C	221	VAL	2.4
1	B	73	ASP	2.4
1	A	210	ALA	2.4
1	A	109	GLN	2.4
1	C	121	PRO	2.4
1	C	45	LYS	2.4
1	D	206	LYS	2.4
1	D	141	LEU	2.4
1	C	149	ARG	2.4
1	C	87	SER	2.4
1	A	194	ALA	2.4
1	A	68	THR	2.4
1	B	237	THR	2.4
1	A	52	SER	2.4
1	C	233	LEU	2.4
1	C	162	HIS	2.4
1	D	233	LEU	2.4
1	B	196	ALA	2.4
1	B	166	TYR	2.4
1	A	85	GLU	2.3
1	A	228	SER	2.3
1	A	53	VAL	2.3
1	A	160	ARG	2.3
1	C	77	LYS	2.3
1	A	192	TYR	2.3
1	A	229	PHE	2.3
1	B	161	THR	2.3
1	C	228	SER	2.3
1	C	193	HIS	2.3
1	A	120	GLU	2.3
1	D	69	GLN	2.3
1	D	70	GLU	2.3
1	A	83	ARG	2.3
1	C	211	LEU	2.3
1	B	225	PHE	2.3
1	D	138	GLN	2.3
1	A	145	GLY	2.3
1	A	164	ALA	2.3
1	B	110	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	125	GLU	2.3
1	C	84	GLN	2.3
1	C	109	GLN	2.3
1	D	223	GLU	2.3
1	A	106	LYS	2.3
1	B	206	LYS	2.3
1	A	63	GLN	2.3
1	B	184	ASN	2.2
1	D	202	THR	2.2
1	A	65	GLY	2.2
1	A	143	PRO	2.2
1	D	82	LEU	2.2
1	A	199	HIS	2.2
1	C	151	ARG	2.2
1	A	127	GLN	2.2
1	B	182	LYS	2.2
1	B	134	LEU	2.2
1	D	197	THR	2.2
1	B	190	ALA	2.2
1	D	144	LEU	2.2
1	A	116	ARG	2.2
1	D	83	ARG	2.2
1	D	196	ALA	2.2
1	C	195	LYS	2.2
1	A	146	GLU	2.2
1	C	163	LEU	2.2
1	B	102	ASP	2.2
1	C	131	ARG	2.2
1	A	155	HIS	2.2
1	C	75	LEU	2.2
1	C	133	LYS	2.2
1	B	84	GLN	2.2
1	B	183	GLU	2.2
1	B	119	VAL	2.2
1	C	53	VAL	2.2
1	A	148	MET	2.2
1	C	112	MET	2.2
1	A	182	LYS	2.1
1	D	75	LEU	2.1
1	A	197	THR	2.1
1	B	197	THR	2.1
1	D	172	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	46	LEU	2.1
1	C	74	ASN	2.1
1	A	56	THR	2.1
1	D	115	TYR	2.1
1	C	78	GLU	2.1
1	B	133	LYS	2.1
1	D	96	LYS	2.1
1	A	171	ARG	2.1
1	C	169	GLU	2.1
1	D	152	ALA	2.1
1	B	170	LEU	2.1
1	B	203	LEU	2.1
1	C	153	ARG	2.1
1	C	173	ARG	2.1
1	B	167	SER	2.1
1	C	167	SER	2.1
1	D	132	GLN	2.1
1	D	222	LEU	2.1
1	D	151	ARG	2.1
1	D	166	TYR	2.1
1	D	81	GLY	2.1
1	A	111	GLU	2.1
1	B	123	ARG	2.1
1	C	177	ARG	2.1
1	D	131	ARG	2.1
1	A	133	LYS	2.1
1	C	129	GLY	2.1
1	B	191	GLU	2.1
1	A	150	ASP	2.0
1	D	103	ASP	2.0
1	A	176	ALA	2.0
1	B	108	TRP	2.0
1	D	110	GLU	2.0
1	D	113	GLU	2.0
1	C	123	ARG	2.0
1	A	134	LEU	2.0
1	C	104	PHE	2.0
1	D	73	ASP	2.0
1	B	143	PRO	2.0
1	D	85	GLU	2.0
1	C	106	LYS	2.0
1	A	130	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	130	ALA	2.0
1	A	103	ASP	2.0
1	D	199	HIS	2.0
1	D	97	VAL	2.0
1	D	153	ARG	2.0
1	A	141	LEU	2.0
1	A	159	LEU	2.0
1	C	201	SER	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 oligosaccharides 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.