



Full wwPDB X-ray Structure Validation Report i

Oct 28, 2024 – 06:31 PM JST

PDB ID : 9JI0
Title : 3-Hydroxybutyryl-CoA dehydrogenase
Authors : Yang, J.W.; Jeon, H.J.; Park, S.H.; Jang, S.H.; Park, J.A.; Kim, S.H.; Hwang, K.Y.
Deposited on : 2024-09-10
Resolution : 2.69 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

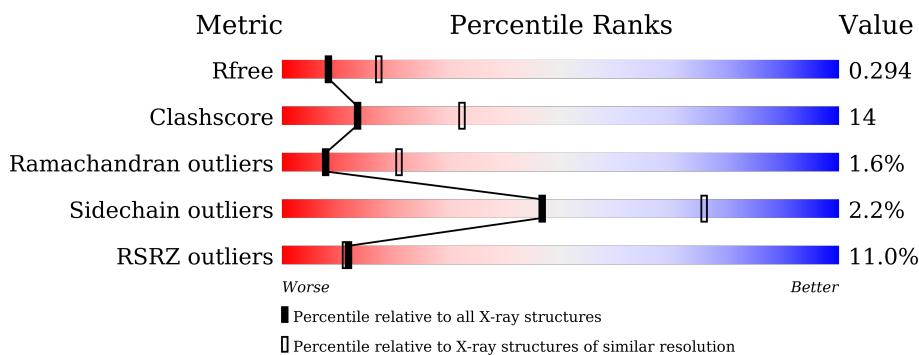
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

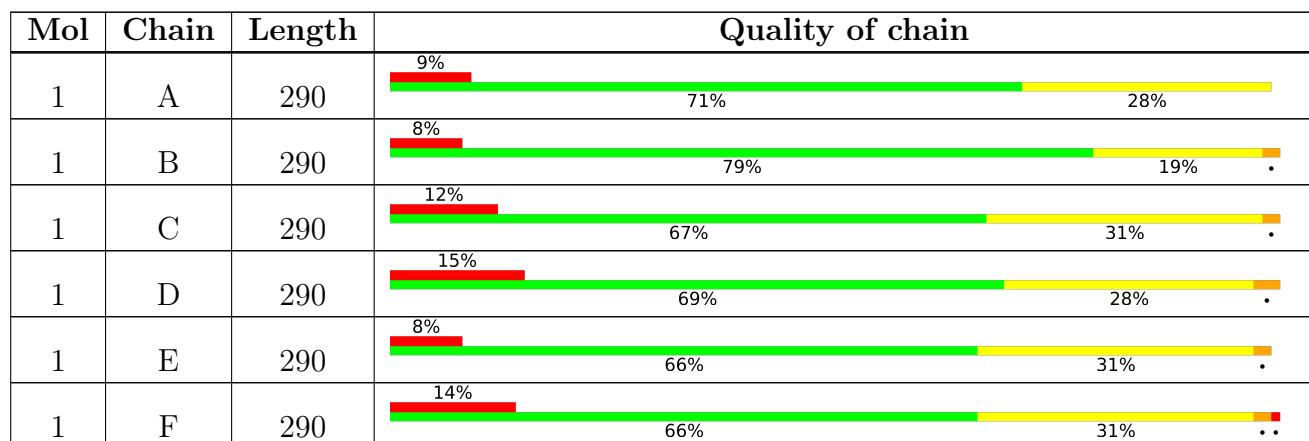
The reported resolution of this entry is 2.69 Å.

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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.



2 Entry composition [\(i\)](#)

There is only 1 type of molecule in this entry. The entry contains 12930 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.

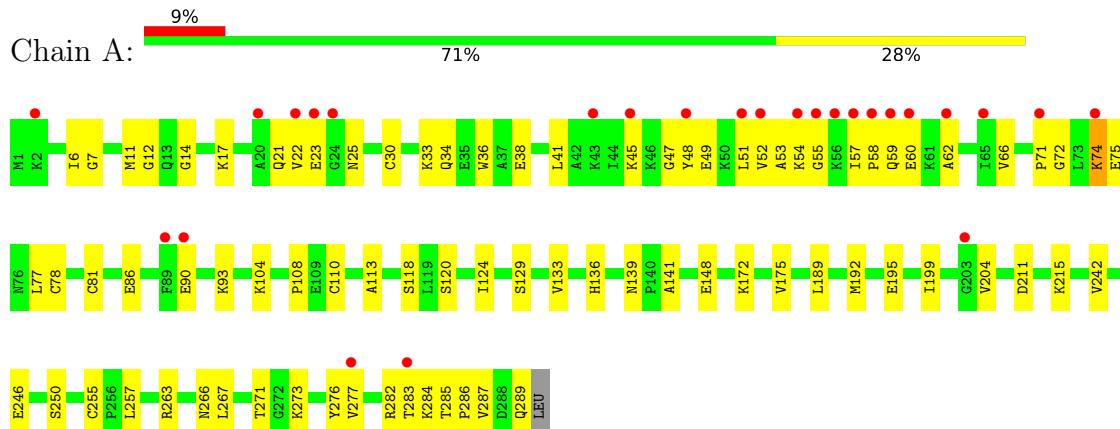
- Molecule 1 is a protein called 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2155	1368	363	404	20	0	0	0
1	B	289	2155	1368	363	404	20	0	0	0
1	C	289	2155	1368	363	404	20	0	0	0
1	D	289	2155	1368	363	404	20	0	0	0
1	E	289	2155	1368	363	404	20	0	0	0
1	F	289	2155	1368	363	404	20	0	0	0

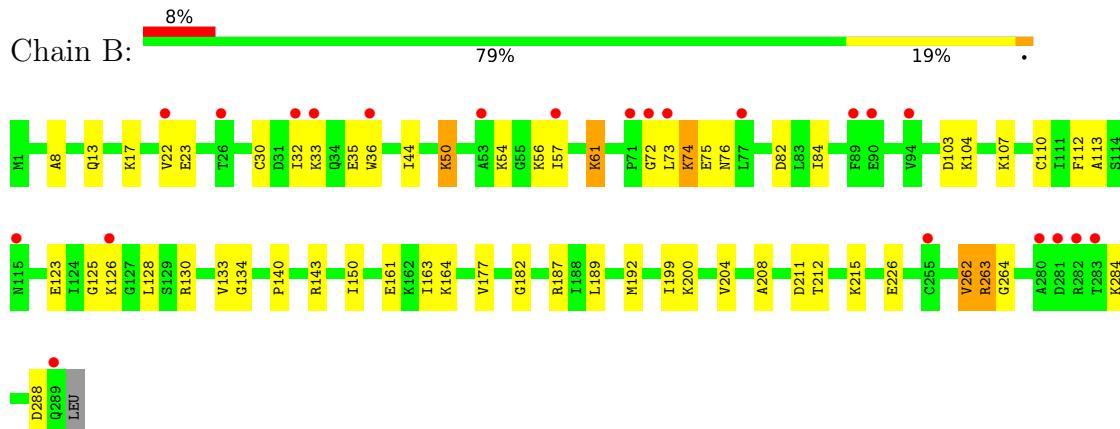
3 Residue-property plots (i)

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: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



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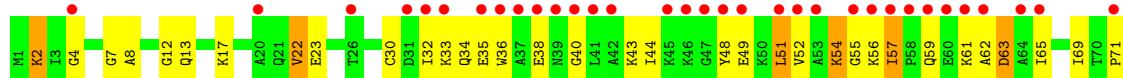




K162	I163	I164	E165	I166	S167	V168	A169	K172	R187	I188	L189	I190	P191	M192	I199	R200	M201	V204	A208	T212	A213	M214	K215	N219	L237	A238	I239	V242	E246	Y252	P256	R259	K273	V277	Y278	A280	D281	R282	T283	K284	Q289
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

LEU

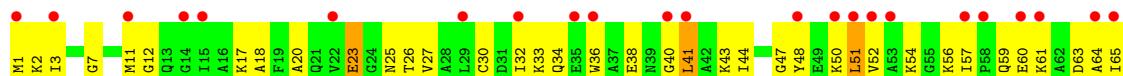
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



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4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.66 Å 126.61 Å 108.09 Å 90.00° 110.19° 90.00°	Depositor
Resolution (Å)	48.04 – 2.69 48.04 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.04-2.69) 98.1 (48.04-2.69)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.27 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (1.17rc1_3605: ????)	Depositor
R , R_{free}	0.246 , 0.294 0.246 , 0.294	Depositor DCC
R_{free} test set	59563 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.4	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12930	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	0/2186	0.62	0/2946
1	B	0.56	1/2186 (0.0%)	0.67	2/2946 (0.1%)
1	C	0.59	4/2186 (0.2%)	0.66	1/2946 (0.0%)
1	D	0.47	0/2186	0.61	2/2946 (0.1%)
1	E	0.55	3/2186 (0.1%)	0.67	4/2946 (0.1%)
1	F	0.51	2/2186 (0.1%)	0.64	2/2946 (0.1%)
All	All	0.53	10/13116 (0.1%)	0.64	11/17676 (0.1%)

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	F	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	LYS	CE-NZ	12.64	1.80	1.49
1	E	109	GLU	CB-CG	10.56	1.72	1.52
1	E	109	GLU	CD-OE1	7.83	1.34	1.25
1	C	33	LYS	CB-CG	7.80	1.73	1.52
1	F	104	LYS	CE-NZ	-6.20	1.33	1.49
1	C	33	LYS	CD-CE	5.84	1.65	1.51
1	B	262	VAL	CB-CG2	5.53	1.64	1.52
1	F	104	LYS	CG-CD	-5.19	1.34	1.52
1	E	107	LYS	CD-CE	-5.19	1.38	1.51
1	C	33	LYS	CG-CD	5.14	1.70	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	126	LYS	CD-CE-NZ	-11.18	85.98	111.70
1	E	109	GLU	OE1-CD-OE2	10.22	135.57	123.30
1	B	263	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	E	109	GLU	CA-CB-CG	7.50	129.91	113.40
1	E	109	GLU	CG-CD-OE1	-7.31	103.68	118.30
1	C	33	LYS	CA-CB-CG	-6.14	99.88	113.40
1	E	109	GLU	CB-CG-CD	-5.98	98.06	114.20
1	D	57	ILE	CG1-CB-CG2	-5.90	98.41	111.40
1	F	126	LYS	CB-CG-CD	-5.39	97.57	111.60
1	D	51	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	263	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	178	ASN	Peptide

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	2155	0	2220	59	0
1	B	2155	0	2220	42	1
1	C	2155	0	2220	67	0
1	D	2155	0	2220	84	0
1	E	2155	0	2220	72	0
1	F	2155	0	2220	83	1
All	All	12930	0	13320	378	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LYS:NZ	1:C:33:LYS:CE	1.80	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ILE:HD11	1:D:61:LYS:CD	1.70	1.22
1:D:57:ILE:CD1	1:D:61:LYS:HD2	1.71	1.20
1:E:32:ILE:HD12	1:E:33:LYS:HG3	1.37	1.07
1:E:73:LEU:HD12	1:E:74:LYS:O	1.59	1.03
1:C:34:GLN:OE1	1:C:72:GLY:HA2	1.63	0.98
1:C:34:GLN:CD	1:C:72:GLY:HA2	1.88	0.94
1:B:73:LEU:HD12	1:B:74:LYS:O	1.69	0.93
1:C:51:LEU:HD23	1:C:56:LYS:HE2	1.50	0.91
1:A:266:ASN:HD21	1:E:154:ASN:HD21	1.18	0.91
1:E:32:ILE:HD12	1:E:33:LYS:CG	2.02	0.89
1:D:32:ILE:HD13	1:D:33:LYS:NZ	1.87	0.89
1:A:108:PRO:HB2	1:B:57:ILE:HD12	1.52	0.88
1:D:32:ILE:HD13	1:D:33:LYS:HZ2	1.36	0.88
1:F:54:LYS:HB2	1:F:56:LYS:HZ2	1.38	0.87
1:A:53:ALA:HB3	1:A:54:LYS:NZ	1.91	0.85
1:D:54:LYS:O	1:D:56:LYS:N	2.10	0.85
1:C:34:GLN:OE1	1:C:72:GLY:CA	2.27	0.81
1:D:34:GLN:O	1:D:38:GLU:N	2.15	0.78
1:A:53:ALA:HB3	1:A:54:LYS:HZ2	1.47	0.78
1:B:82:ASP:OD1	1:B:107:LYS:NZ	2.17	0.78
1:C:145:LYS:HA	1:C:172:LYS:HD2	1.65	0.77
1:E:45:LYS:HG2	1:E:66:VAL:HG11	1.66	0.77
1:D:32:ILE:CD1	1:D:33:LYS:HD3	2.15	0.77
1:E:53:ALA:O	1:E:55:GLY:N	2.17	0.76
1:D:283:THR:HG22	1:D:284:LYS:H	1.50	0.76
1:F:118:SER:HB2	1:F:242:VAL:HG21	1.68	0.76
1:F:54:LYS:HB2	1:F:56:LYS:NZ	2.00	0.75
1:D:32:ILE:HD12	1:D:33:LYS:HD3	1.69	0.75
1:E:99:PHE:HB3	1:E:128:LEU:HD21	1.69	0.75
1:D:99:PHE:HB3	1:D:128:LEU:HD21	1.70	0.73
1:F:201:MET:HE1	1:F:256:PRO:HD2	1.71	0.73
1:B:50:LYS:O	1:B:50:LYS:NZ	2.22	0.72
1:C:154:ASN:HD21	1:F:266:ASN:HD21	1.36	0.72
1:D:32:ILE:CD1	1:D:33:LYS:NZ	2.51	0.72
1:F:32:ILE:HG13	1:F:36:TRP:CD1	2.25	0.72
1:E:86:GLU:OE2	1:E:95:LYS:NZ	2.19	0.71
1:D:246:GLU:OE2	1:E:263:ARG:NH2	2.20	0.71
1:F:1:MET:HG3	1:F:3:ILE:HD11	1.74	0.70
1:B:50:LYS:NZ	1:B:54:LYS:HG3	2.07	0.69
1:D:212:THR:HA	1:D:215:LYS:HE2	1.74	0.69
1:F:215:LYS:HD3	1:F:222:MET:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HG3	1:A:277:VAL:HG12	1.75	0.69
1:D:57:ILE:HD11	1:D:61:LYS:HD2	0.80	0.69
1:D:121:ILE:HD13	1:D:150:ILE:HG21	1.75	0.68
1:C:153:CYS:SG	1:F:266:ASN:ND2	2.67	0.68
1:D:4:GLY:HA3	1:D:84:ILE:HD13	1.76	0.68
1:B:226:GLU:OE2	1:B:284:LYS:NZ	2.27	0.68
1:D:121:ILE:HD12	1:D:121:ILE:H	1.59	0.67
1:C:134:GLY:HA3	1:C:150:ILE:HB	1.75	0.67
1:A:263:ARG:NH2	1:E:246:GLU:OE2	2.19	0.67
1:F:41:LEU:HD13	1:F:71:PRO:HD3	1.78	0.66
1:E:199:ILE:HG23	1:E:204:VAL:HB	1.77	0.66
1:C:89:PHE:O	1:C:91:ASP:N	2.28	0.66
1:E:251:LYS:HD3	1:E:252:TYR:CZ	2.31	0.66
1:B:74:LYS:O	1:B:76:ASN:N	2.29	0.65
1:A:246:GLU:OE2	1:D:263:ARG:NH2	2.30	0.65
1:F:176:GLN:HE21	1:F:178:ASN:HD21	1.43	0.65
1:F:59:GLN:NE2	1:F:63:ASP:OD1	2.25	0.64
1:E:32:ILE:CD1	1:E:33:LYS:HG3	2.22	0.64
1:D:17:LYS:HD3	1:D:48:TYR:HE2	1.62	0.64
1:E:103:ASP:OD1	1:E:129:SER:OG	2.15	0.64
1:D:122:THR:OG1	1:D:179:GLU:OE1	2.15	0.64
1:C:86:GLU:HG2	1:C:99:PHE:CE2	2.33	0.63
1:B:50:LYS:HZ1	1:B:54:LYS:HG3	1.63	0.63
1:A:266:ASN:HD21	1:E:154:ASN:ND2	1.94	0.63
1:D:40:GLY:O	1:D:44:ILE:HG13	1.99	0.63
1:B:8:ALA:O	1:B:13:GLN:NE2	2.28	0.63
1:D:109:GLU:OE2	1:D:109:GLU:N	2.31	0.62
1:B:262:VAL:C	1:B:264:GLY:H	2.02	0.62
1:E:54:LYS:HB2	1:E:56:LYS:HG2	1.82	0.62
1:B:33:LYS:HB2	1:B:36:TRP:CD1	2.35	0.61
1:A:189:LEU:O	1:A:192:MET:HB2	2.00	0.61
1:F:48:TYR:HE2	1:F:65:ILE:HG21	1.65	0.61
1:F:104:LYS:HG3	1:F:104:LYS:O	1.99	0.61
1:C:189:LEU:O	1:C:192:MET:HB2	2.01	0.60
1:A:17:LYS:O	1:A:21:GLN:HG3	2.00	0.60
1:C:109:GLU:N	1:C:109:GLU:OE2	2.32	0.60
1:F:89:PHE:O	1:F:91:ASP:N	2.34	0.60
1:D:199:ILE:HG23	1:D:204:VAL:HB	1.83	0.60
1:E:189:LEU:O	1:E:192:MET:HB2	2.02	0.60
1:D:95:LYS:HE2	1:D:119:LEU:HD12	1.84	0.59
1:D:133:VAL:HG11	1:D:163:ILE:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:SER:OG	1:B:61:LYS:HE2	2.02	0.59
1:F:189:LEU:O	1:F:192:MET:HB2	2.02	0.59
1:D:107:LYS:O	1:D:130:ARG:NH1	2.31	0.59
1:F:283:THR:HG22	1:F:284:LYS:H	1.67	0.59
1:A:141:ALA:O	1:A:172:LYS:NZ	2.30	0.59
1:F:51:LEU:HA	1:F:56:LYS:NZ	2.18	0.59
1:C:103:ASP:O	1:C:130:ARG:NH2	2.36	0.58
1:D:32:ILE:HD12	1:D:33:LYS:N	2.17	0.58
1:D:32:ILE:HD11	1:D:36:TRP:CD1	2.38	0.58
1:E:253:ARG:NH2	1:F:249:ASP:OD2	2.33	0.58
1:F:51:LEU:HA	1:F:56:LYS:HZ1	1.68	0.58
1:B:54:LYS:HB3	1:B:56:LYS:HD2	1.86	0.58
1:B:134:GLY:HA3	1:B:150:ILE:HB	1.85	0.58
1:B:211:ASP:O	1:B:215:LYS:HG2	2.03	0.57
1:F:134:GLY:HA3	1:F:150:ILE:HB	1.86	0.57
1:B:125:GLY:HA2	1:B:128:LEU:HD13	1.86	0.57
1:C:201:MET:HE1	1:C:256:PRO:HB2	1.87	0.57
1:E:221:PRO:HG3	1:F:219:ASN:HB3	1.86	0.57
1:F:125:GLY:HA2	1:F:128:LEU:HD13	1.86	0.57
1:A:53:ALA:CB	1:A:54:LYS:HZ2	2.15	0.57
1:D:40:GLY:HA2	1:D:43:LYS:HD2	1.87	0.57
1:F:33:LYS:O	1:F:36:TRP:HB2	2.05	0.57
1:B:123:GLU:HG3	1:B:126:LYS:NZ	2.19	0.57
1:F:103:ASP:OD1	1:F:129:SER:OG	2.21	0.56
1:E:283:THR:HG22	1:E:284:LYS:H	1.70	0.56
1:D:89:PHE:O	1:D:95:LYS:NZ	2.36	0.56
1:A:199:ILE:HG23	1:A:204:VAL:HB	1.86	0.56
1:C:47:GLY:O	1:C:51:LEU:HD12	2.05	0.56
1:C:78:CYS:HA	1:C:81:CYS:SG	2.45	0.56
1:F:54:LYS:HD3	1:F:56:LYS:HZ1	1.71	0.56
1:C:75:GLU:HG3	1:C:105:ILE:HD11	1.88	0.56
1:D:52:VAL:HA	1:D:57:ILE:O	2.05	0.56
1:A:74:LYS:O	1:A:75:GLU:HB2	2.06	0.56
1:D:277:VAL:HG23	1:D:287:VAL:HG12	1.87	0.55
1:C:154:ASN:HD21	1:F:266:ASN:ND2	2.04	0.55
1:F:136:HIS:HB3	1:F:148:GLU:HB2	1.88	0.55
1:C:30:CYS:HA	1:C:72:GLY:O	2.07	0.55
1:D:132:LEU:O	1:D:155:THR:OG1	2.24	0.55
1:F:59:GLN:O	1:F:63:ASP:N	2.39	0.55
1:F:199:ILE:HG23	1:F:204:VAL:HB	1.88	0.55
1:E:277:VAL:HG23	1:E:287:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:LYS:HD3	1:F:165:GLU:OE1	2.05	0.55
1:A:283:THR:HG22	1:A:284:LYS:H	1.72	0.55
1:E:74:LYS:O	1:E:75:GLU:HB2	2.05	0.55
1:F:34:GLN:HE21	1:F:72:GLY:HA2	1.72	0.55
1:A:266:ASN:ND2	1:E:154:ASN:HD21	1.98	0.55
1:D:78:CYS:HA	1:D:81:CYS:SG	2.46	0.55
1:E:30:CYS:HA	1:E:72:GLY:O	2.07	0.55
1:E:200:LYS:NZ	1:E:288:ASP:OD1	2.23	0.55
1:F:18:ALA:HB2	1:F:142:ASP:HA	1.89	0.55
1:E:22:VAL:HG21	1:E:170:ILE:HG22	1.88	0.55
1:D:22:VAL:HG21	1:D:170:ILE:HG22	1.89	0.54
1:D:207:ILE:N	1:D:288:ASP:OD2	2.24	0.54
1:B:133:VAL:HG11	1:B:163:ILE:HG13	1.88	0.54
1:E:160:VAL:O	1:E:164:LYS:HG3	2.08	0.54
1:A:34:GLN:O	1:A:38:GLU:HG3	2.07	0.54
1:D:35:GLU:HA	1:D:38:GLU:HB2	1.88	0.54
1:D:95:LYS:HD2	1:D:124:ILE:HD13	1.88	0.54
1:E:3:ILE:HD13	1:E:19:PHE:CG	2.42	0.54
1:E:189:LEU:HD21	1:E:227:LEU:HD21	1.89	0.54
1:A:277:VAL:HG23	1:A:285:THR:HB	1.88	0.54
1:D:32:ILE:CD1	1:D:33:LYS:CE	2.85	0.54
1:D:32:ILE:HD13	1:D:33:LYS:HD3	1.90	0.53
1:F:99:PHE:HB3	1:F:128:LEU:HD21	1.91	0.53
1:E:190:ILE:HG13	1:E:239:ILE:HG21	1.90	0.53
1:F:94:VAL:HA	1:F:97:THR:OG1	2.08	0.53
1:B:84:ILE:HG12	1:B:110:CYS:SG	2.48	0.53
1:D:2:LYS:HB2	1:D:81:CYS:HA	1.91	0.53
1:C:40:GLY:O	1:C:44:ILE:HG13	2.08	0.53
1:D:17:LYS:HD3	1:D:48:TYR:CE2	2.41	0.53
1:F:279:ASN:HD22	1:F:283:THR:HB	1.74	0.53
1:A:277:VAL:CG2	1:A:285:THR:HB	2.38	0.53
1:D:51:LEU:C	1:D:57:ILE:HG22	2.29	0.53
1:F:51:LEU:HD23	1:F:56:LYS:HE2	1.92	0.52
1:A:266:ASN:ND2	1:E:153:CYS:SG	2.82	0.52
1:E:278:TYR:HE1	1:E:284:LYS:HD3	1.75	0.52
1:F:27:VAL:CG1	1:F:69:ILE:HG12	2.39	0.52
1:D:73:LEU:HD12	1:D:74:LYS:O	2.10	0.52
1:F:286:PRO:C	1:F:288:ASP:H	2.11	0.52
1:D:208:ALA:O	1:D:212:THR:HG23	2.09	0.52
1:E:216:LEU:HD13	1:F:145:LYS:HG3	1.91	0.52
1:A:246:GLU:CD	1:D:263:ARG:HH22	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASN:ND2	1:F:266:ASN:HD21	2.07	0.51
1:C:199:ILE:HG23	1:C:204:VAL:HB	1.91	0.51
1:E:62:ALA:O	1:E:66:VAL:HG23	2.10	0.51
1:B:199:ILE:HG23	1:B:204:VAL:HB	1.92	0.51
1:C:74:LYS:O	1:C:76:ASN:N	2.42	0.51
1:D:13:GLN:O	1:D:17:LYS:HG3	2.10	0.51
1:B:33:LYS:HB2	1:B:36:TRP:HD1	1.76	0.51
1:F:56:LYS:NZ	1:F:56:LYS:HB2	2.24	0.51
1:A:62:ALA:O	1:A:66:VAL:HG23	2.11	0.51
1:D:74:LYS:O	1:D:76:ASN:N	2.37	0.51
1:F:41:LEU:HA	1:F:44:ILE:HD12	1.92	0.51
1:A:48:TYR:CD1	1:A:51:LEU:HD12	2.46	0.51
1:F:47:GLY:O	1:F:51:LEU:HD12	2.10	0.50
1:D:7:GLY:O	1:D:12:GLY:HA3	2.10	0.50
1:D:33:LYS:O	1:D:36:TRP:HB2	2.11	0.50
1:F:48:TYR:CE2	1:F:65:ILE:HG21	2.45	0.50
1:D:32:ILE:HD12	1:D:33:LYS:CD	2.39	0.50
1:D:51:LEU:HB3	1:D:57:ILE:CG2	2.41	0.50
1:A:6:ILE:HB	1:A:86:GLU:HG2	1.93	0.50
1:A:104:LYS:HB3	1:B:22:VAL:HG13	1.93	0.50
1:A:192:MET:SD	1:C:192:MET:SD	3.09	0.50
1:C:118:SER:HB2	1:C:242:VAL:HG21	1.93	0.50
1:D:189:LEU:O	1:D:192:MET:HB2	2.11	0.50
1:E:164:LYS:O	1:E:168:VAL:HG23	2.12	0.50
1:D:90:GLU:OE1	1:D:118:SER:OG	2.19	0.49
1:C:75:GLU:HG3	1:C:105:ILE:CD1	2.42	0.49
1:D:32:ILE:CD1	1:D:33:LYS:CD	2.86	0.49
1:A:286:PRO:HG2	1:A:289:GLN:HE21	1.77	0.49
1:E:216:LEU:HD22	1:F:145:LYS:HE3	1.93	0.49
1:C:33:LYS:O	1:C:36:TRP:N	2.46	0.49
1:A:47:GLY:O	1:A:51:LEU:HG	2.12	0.49
1:D:40:GLY:O	1:D:43:LYS:HB2	2.13	0.48
1:A:49:GLU:O	1:A:52:VAL:HG12	2.12	0.48
1:E:170:ILE:HG13	1:E:172:LYS:HG2	1.94	0.48
1:F:30:CYS:HA	1:F:72:GLY:O	2.12	0.48
1:D:49:GLU:OE2	1:D:59:GLN:NE2	2.46	0.48
1:D:52:VAL:HG22	1:D:57:ILE:HG23	1.95	0.48
1:F:170:ILE:HG13	1:F:172:LYS:HG2	1.94	0.48
1:A:7:GLY:O	1:A:12:GLY:HA3	2.14	0.48
1:B:113:ALA:HA	1:B:133:VAL:O	2.13	0.47
1:C:111:ILE:HD11	1:C:162:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:PHE:CZ	1:E:255:CYS:HA	2.50	0.47
1:B:208:ALA:O	1:B:212:THR:HG23	2.14	0.47
1:F:23:GLU:C	1:F:25:ASN:H	2.17	0.47
1:E:86:GLU:HG2	1:E:99:PHE:CE2	2.49	0.47
1:D:73:LEU:O	1:D:77:LEU:HD12	2.14	0.47
1:F:11:MET:SD	1:F:139:ASN:HB2	2.55	0.47
1:F:34:GLN:HE21	1:F:72:GLY:CA	2.27	0.47
1:B:150:ILE:HD13	1:B:177:VAL:HB	1.96	0.47
1:E:23:GLU:C	1:E:25:ASN:H	2.18	0.47
1:F:50:LYS:NZ	1:F:54:LYS:HG3	2.30	0.47
1:F:52:VAL:HA	1:F:57:ILE:O	2.14	0.47
1:A:273:LYS:HG3	1:A:277:VAL:CG1	2.44	0.47
1:E:54:LYS:CB	1:E:56:LYS:HG2	2.43	0.47
1:F:56:LYS:HB2	1:F:56:LYS:HZ3	1.79	0.47
1:E:120:SER:O	1:E:124:ILE:HG13	2.14	0.47
1:F:7:GLY:O	1:F:12:GLY:HA3	2.15	0.47
1:F:34:GLN:O	1:F:38:GLU:HG2	2.15	0.47
1:F:126:LYS:HD3	1:F:126:LYS:HA	1.25	0.47
1:A:41:LEU:HD22	1:A:71:PRO:HD3	1.96	0.46
1:A:72:GLY:HA3	1:A:77:LEU:HD11	1.96	0.46
1:C:136:HIS:HB3	1:C:148:GLU:HB2	1.97	0.46
1:D:32:ILE:CD1	1:D:33:LYS:HZ3	2.27	0.46
1:D:170:ILE:HG13	1:D:172:LYS:HG2	1.96	0.46
1:E:41:LEU:HG	1:E:45:LYS:HE3	1.97	0.46
1:E:58:PRO:HD2	1:E:61:LYS:HD3	1.96	0.46
1:E:162:LYS:HA	1:E:162:LYS:HD3	1.69	0.46
1:F:51:LEU:HD23	1:F:56:LYS:CE	2.45	0.46
1:E:207:ILE:HG23	1:E:225:LEU:HD12	1.97	0.46
1:C:33:LYS:HA	1:C:33:LYS:HD3	1.42	0.46
1:C:98:THR:O	1:C:102:LEU:HG	2.16	0.46
1:D:59:GLN:HG3	1:D:63:ASP:OD1	2.16	0.46
1:E:89:PHE:O	1:E:91:ASP:N	2.46	0.46
1:F:17:LYS:HB2	1:F:142:ASP:HB3	1.97	0.46
1:A:53:ALA:CB	1:A:54:LYS:NZ	2.72	0.46
1:C:102:LEU:HA	1:C:105:ILE:HB	1.98	0.46
1:C:120:SER:O	1:C:124:ILE:HG13	2.15	0.46
1:D:32:ILE:HD12	1:D:33:LYS:H	1.81	0.46
1:A:14:GLY:C	1:A:141:ALA:HB3	2.36	0.46
1:A:81:CYS:O	1:A:110:CYS:HB2	2.16	0.46
1:A:113:ALA:HA	1:A:133:VAL:O	2.16	0.46
1:A:195:GLU:OE2	1:C:252:TYR:OH	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HG13	1:B:33:LYS:H	1.81	0.46
1:C:48:TYR:O	1:C:52:VAL:HG23	2.15	0.46
1:E:195:GLU:OE2	1:F:187:ARG:NE	2.35	0.46
1:A:136:HIS:HB3	1:A:148:GLU:HB2	1.97	0.46
1:E:32:ILE:HD12	1:E:33:LYS:HG2	1.92	0.46
1:F:33:LYS:HA	1:F:73:LEU:HD23	1.98	0.46
1:A:255:CYS:SG	1:A:257:LEU:HB3	2.56	0.45
1:A:286:PRO:HG2	1:A:289:GLN:NE2	2.32	0.45
1:F:164:LYS:HG2	1:F:174:PRO:HB2	1.99	0.45
1:A:78:CYS:HA	1:A:81:CYS:SG	2.57	0.45
1:D:211:ASP:O	1:D:215:LYS:HG2	2.17	0.45
1:C:139:ASN:ND2	1:C:140:PRO:HA	2.32	0.45
1:D:48:TYR:HA	1:D:51:LEU:HB2	1.99	0.45
1:A:60:GLU:OE1	1:A:60:GLU:N	2.50	0.45
1:B:123:GLU:HG3	1:B:126:LYS:HZ2	1.82	0.45
1:E:30:CYS:HB3	1:E:73:LEU:HA	1.99	0.45
1:D:4:GLY:HA3	1:D:84:ILE:CD1	2.45	0.44
1:C:190:ILE:HG13	1:C:239:ILE:HG21	1.99	0.44
1:F:2:LYS:HA	1:F:26:THR:O	2.17	0.44
1:A:23:GLU:C	1:A:25:ASN:H	2.21	0.44
1:A:11:MET:SD	1:A:139:ASN:HB2	2.57	0.44
1:D:54:LYS:HB2	1:D:54:LYS:HE2	1.76	0.44
1:D:113:ALA:HA	1:D:133:VAL:O	2.18	0.44
1:C:42:ALA:O	1:C:46:LYS:HG3	2.18	0.44
1:C:246:GLU:OE2	1:F:263:ARG:NH2	2.39	0.44
1:D:30:CYS:HA	1:D:72:GLY:O	2.18	0.44
1:A:267:LEU:HG	1:A:271:THR:HG21	1.98	0.44
1:F:20:ALA:O	1:F:65:ILE:HG12	2.18	0.44
1:C:284:LYS:HZ2	1:C:284:LYS:HB3	1.83	0.44
1:C:112:PHE:HB3	1:C:132:LEU:HD13	2.00	0.43
1:D:51:LEU:HB3	1:D:57:ILE:HG22	1.99	0.43
1:D:273:LYS:HG3	1:D:277:VAL:HG22	1.99	0.43
1:E:78:CYS:HA	1:E:81:CYS:SG	2.58	0.43
1:F:178:ASN:HD22	1:F:178:ASN:N	2.16	0.43
1:B:140:PRO:HG2	1:B:143:ARG:HB2	1.99	0.43
1:F:48:TYR:HE2	1:F:65:ILE:CG2	2.31	0.43
1:A:33:LYS:HD2	1:A:36:TRP:CE2	2.53	0.43
1:A:57:ILE:HG12	1:A:58:PRO:O	2.18	0.43
1:A:120:SER:O	1:A:124:ILE:HG13	2.18	0.43
1:E:207:ILE:HG23	1:E:225:LEU:CD1	2.48	0.43
1:E:47:GLY:O	1:E:51:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LYS:O	1:C:21:GLN:HG3	2.18	0.43
1:D:32:ILE:HD13	1:D:33:LYS:CD	2.48	0.43
1:F:215:LYS:HG2	1:F:220:HIS:O	2.19	0.43
1:B:33:LYS:HB3	1:B:35:GLU:HG2	2.00	0.42
1:C:34:GLN:HE21	1:C:34:GLN:HB3	1.66	0.42
1:C:164:LYS:O	1:C:168:VAL:HG23	2.20	0.42
1:D:65:ILE:O	1:D:69:ILE:HG13	2.19	0.42
1:E:1:MET:O	1:E:25:ASN:HA	2.19	0.42
1:F:33:LYS:O	1:F:36:TRP:N	2.47	0.42
1:B:30:CYS:HA	1:B:72:GLY:O	2.19	0.42
1:B:189:LEU:O	1:B:192:MET:HB2	2.19	0.42
1:E:86:GLU:HG3	1:E:114:SER:HA	2.00	0.42
1:C:90:GLU:HA	1:C:95:LYS:HE2	2.00	0.42
1:C:237:LEU:HD11	1:C:259:ARG:NH1	2.34	0.42
1:D:131:PRO:HB3	1:D:156:PRO:CD	2.48	0.42
1:F:1:MET:HG3	1:F:3:ILE:CD1	2.45	0.42
1:F:109:GLU:CD	1:F:109:GLU:H	2.23	0.42
1:B:161:GLU:OE1	1:B:164:LYS:HE2	2.19	0.42
1:B:164:LYS:HE3	1:B:164:LYS:HB3	1.70	0.42
1:C:246:GLU:CD	1:F:263:ARG:HH22	2.21	0.42
1:E:112:PHE:O	1:E:133:VAL:HG12	2.19	0.42
1:D:121:ILE:H	1:D:121:ILE:CD1	2.29	0.42
1:C:32:ILE:O	1:C:33:LYS:HE2	2.18	0.42
1:E:176:GLN:O	1:F:205:SER:HB2	2.19	0.42
1:E:192:MET:SD	1:F:192:MET:SD	3.17	0.42
1:A:211:ASP:O	1:A:215:LYS:HG2	2.20	0.42
1:B:182:GLY:HA3	1:B:187:ARG:HB2	2.01	0.42
1:F:282:ARG:O	1:F:282:ARG:HG3	2.19	0.42
1:A:52:VAL:HG21	1:A:59:GLN:HB2	2.01	0.42
1:C:2:LYS:N	1:C:82:ASP:OD1	2.30	0.42
1:D:134:GLY:HA3	1:D:150:ILE:HB	2.00	0.42
1:A:54:LYS:HA	1:A:54:LYS:HD3	1.82	0.42
1:E:59:GLN:O	1:E:59:GLN:HG3	2.19	0.42
1:C:8:ALA:HA	1:C:29:LEU:HD11	2.01	0.42
1:C:86:GLU:HG2	1:C:99:PHE:CZ	2.54	0.42
1:C:215:LYS:O	1:C:219:ASN:HA	2.20	0.42
1:D:4:GLY:CA	1:D:84:ILE:HD13	2.47	0.42
1:E:13:GLN:O	1:E:17:LYS:HG3	2.19	0.42
1:F:61:LYS:O	1:F:64:ALA:N	2.53	0.42
1:B:17:LYS:HD3	1:B:44:ILE:HG12	2.02	0.41
1:D:99:PHE:CE1	1:D:112:PHE:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASP:OD2	1:E:143:ARG:HG3	2.20	0.41
1:B:103:ASP:O	1:B:130:ARG:NH2	2.50	0.41
1:D:8:ALA:O	1:D:13:GLN:NE2	2.37	0.41
1:D:122:THR:HG22	1:E:264:GLY:CA	2.50	0.41
1:A:118:SER:HB2	1:A:242:VAL:HG21	2.01	0.41
1:B:33:LYS:HG3	1:B:36:TRP:HD1	1.84	0.41
1:C:208:ALA:O	1:C:212:THR:HG23	2.21	0.41
1:F:40:GLY:O	1:F:44:ILE:HG13	2.21	0.41
1:C:282:ARG:HE	1:C:282:ARG:HA	1.86	0.41
1:D:75:GLU:HA	1:D:105:ILE:HG21	2.02	0.41
1:E:211:ASP:OD2	1:E:226:GLU:HG3	2.20	0.41
1:F:2:LYS:HG3	1:F:26:THR:OG1	2.20	0.41
1:F:215:LYS:HD3	1:F:222:MET:CA	2.48	0.41
1:B:107:LYS:HE2	1:B:107:LYS:HB2	1.81	0.41
1:C:38:GLU:HG3	1:C:71:PRO:HG3	2.03	0.41
1:E:57:ILE:HD12	1:E:57:ILE:HA	1.86	0.41
1:F:50:LYS:HA	1:F:50:LYS:HD2	1.75	0.41
1:F:50:LYS:HG3	1:F:54:LYS:HD2	2.03	0.41
1:C:137:PHE:CD2	1:C:141:ALA:HB1	2.54	0.41
1:D:48:TYR:HB3	1:D:62:ALA:HB1	2.03	0.41
1:E:8:ALA:O	1:E:13:GLN:NE2	2.43	0.41
1:E:52:VAL:HA	1:E:57:ILE:O	2.21	0.41
1:E:136:HIS:HD1	1:E:183:PHE:HD2	1.69	0.41
1:A:277:VAL:HG13	1:A:287:VAL:HG12	2.02	0.41
1:C:50:LYS:HE2	1:C:50:LYS:HB2	1.81	0.41
1:E:34:GLN:HG2	1:E:72:GLY:HA2	2.02	0.41
1:B:200:LYS:NZ	1:B:288:ASP:OD1	2.43	0.41
1:C:11:MET:SD	1:C:139:ASN:HB2	2.60	0.41
1:C:273:LYS:HG3	1:C:277:VAL:HG12	2.03	0.41
1:C:273:LYS:HG3	1:C:277:VAL:CG1	2.51	0.41
1:E:48:TYR:O	1:E:52:VAL:HG23	2.21	0.41
1:F:93:LYS:O	1:F:93:LYS:HG2	2.21	0.41
1:D:49:GLU:CD	1:D:59:GLN:HE22	2.24	0.41
1:E:190:ILE:HB	1:E:191:PRO:HD3	2.02	0.41
1:A:199:ILE:HD11	1:C:187:ARG:HD3	2.02	0.40
1:B:104:LYS:HA	1:B:104:LYS:HD3	1.80	0.40
1:C:166:ILE:O	1:C:169:ALA:N	2.53	0.40
1:D:95:LYS:HD2	1:D:124:ILE:CD1	2.51	0.40
1:A:30:CYS:HA	1:A:72:GLY:O	2.21	0.40
1:F:95:LYS:HB3	1:F:95:LYS:HZ2	1.85	0.40
1:A:276:TYR:HB3	1:A:284:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:HB2	1:B:36:TRP:HB2	2.03	0.40
1:B:112:PHE:CD1	1:B:130:ARG:HD2	2.56	0.40
1:C:133:VAL:HG11	1:C:163:ILE:HG13	2.04	0.40
1:E:118:SER:HB2	1:E:242:VAL:HG21	2.03	0.40
1:C:52:VAL:HG11	1:C:59:GLN:OE1	2.22	0.40
1:E:173:ASN:N	1:E:173:ASN:OD1	2.55	0.40
1:A:175:VAL:HG21	1:C:213:ALA:HB2	2.03	0.40
1:C:155:THR:HA	1:C:156:PRO:HD3	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:NH2	1:F:246:GLU:OE2[2_444]	2.09	0.11

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	287/290 (99%)	262 (91%)	22 (8%)	3 (1%)	13 33
1	B	287/290 (99%)	266 (93%)	18 (6%)	3 (1%)	13 33
1	C	287/290 (99%)	265 (92%)	17 (6%)	5 (2%)	7 20
1	D	287/290 (99%)	272 (95%)	10 (4%)	5 (2%)	7 20
1	E	287/290 (99%)	266 (93%)	17 (6%)	4 (1%)	9 24
1	F	287/290 (99%)	258 (90%)	22 (8%)	7 (2%)	5 13
All	All	1722/1740 (99%)	1589 (92%)	106 (6%)	27 (2%)	8 21

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	LYS
1	C	90	GLU
1	D	22	VAL
1	D	55	GLY
1	E	53	ALA
1	F	90	GLU
1	B	23	GLU
1	C	71	PRO
1	C	74	LYS
1	C	126	LYS
1	D	23	GLU
1	D	74	LYS
1	E	23	GLU
1	E	74	LYS
1	F	74	LYS
1	F	88	ALA
1	F	126	LYS
1	A	55	GLY
1	B	75	GLU
1	E	54	LYS
1	F	23	GLU
1	A	74	LYS
1	F	60	GLU
1	C	282	ARG
1	F	287	VAL
1	D	71	PRO
1	A	22	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	228/231 (99%)	223 (98%)	5 (2%)	47 76
1	B	228/231 (99%)	226 (99%)	2 (1%)	75 90
1	C	228/231 (99%)	225 (99%)	3 (1%)	65 85
1	D	228/231 (99%)	222 (97%)	6 (3%)	41 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	228/231 (99%)	223 (98%)	5 (2%)	47 76
1	F	228/231 (99%)	219 (96%)	9 (4%)	27 56
All	All	1368/1386 (99%)	1338 (98%)	30 (2%)	47 76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	90	GLU
1	A	93	LYS
1	A	250	SER
1	A	282	ARG
1	B	50	LYS
1	B	61	LYS
1	C	33	LYS
1	C	48	TYR
1	C	143	ARG
1	D	2	LYS
1	D	54	LYS
1	D	63	ASP
1	D	93	LYS
1	D	215	LYS
1	D	282	ARG
1	E	2	LYS
1	E	86	GLU
1	E	109	GLU
1	E	173	ASN
1	E	282	ARG
1	F	41	LEU
1	F	43	LYS
1	F	51	LEU
1	F	89	PHE
1	F	109	GLU
1	F	126	LYS
1	F	161	GLU
1	F	178	ASN
1	F	205	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	289	GLN
1	B	34	GLN
1	B	154	ASN
1	C	139	ASN
1	E	220	HIS
1	F	34	GLN
1	F	96	GLN
1	F	178	ASN
1	F	220	HIS
1	F	266	ASN
1	F	279	ASN

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 [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/290 (99%)	0.51	26 (8%) 17 15	26, 45, 87, 102	0
1	B	289/290 (99%)	0.41	22 (7%) 21 19	24, 46, 69, 93	0
1	C	289/290 (99%)	0.61	34 (11%) 10 10	27, 44, 84, 103	0
1	D	289/290 (99%)	0.84	43 (14%) 7 6	28, 47, 85, 114	0
1	E	289/290 (99%)	0.63	23 (7%) 20 18	29, 51, 77, 91	0
1	F	289/290 (99%)	0.83	42 (14%) 7 6	30, 58, 96, 114	0
All	All	1734/1740 (99%)	0.64	190 (10%) 12 11	24, 48, 86, 114	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	VAL	7.5
1	D	53	ALA	7.4
1	D	57	ILE	7.4
1	D	56	LYS	7.0
1	D	48	TYR	6.6
1	D	55	GLY	6.2
1	C	280	ALA	5.8
1	A	48	TYR	5.3
1	F	78	CYS	5.3
1	E	280	ALA	5.3
1	D	41	LEU	5.3
1	D	60	GLU	5.1
1	C	4	GLY	5.0
1	C	33	LYS	4.9
1	A	55	GLY	4.8
1	D	58	PRO	4.6
1	B	90	GLU	4.5
1	C	89	PHE	4.5
1	D	36	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	89	PHE	4.4
1	F	53	ALA	4.4
1	C	36	TRP	4.3
1	A	56	LYS	4.2
1	F	52	VAL	4.1
1	D	89	PHE	4.1
1	E	281	ASP	4.0
1	E	32	ILE	4.0
1	D	32	ILE	3.9
1	A	283	THR	3.9
1	A	62	ALA	3.8
1	D	42	ALA	3.8
1	A	58	PRO	3.8
1	C	32	ILE	3.8
1	C	74	LYS	3.8
1	F	40	GLY	3.7
1	E	283	THR	3.7
1	D	280	ALA	3.6
1	E	78	CYS	3.6
1	C	38	GLU	3.5
1	A	57	ILE	3.4
1	F	283	THR	3.4
1	D	35	GLU	3.4
1	D	45	LYS	3.4
1	B	89	PHE	3.3
1	E	279	ASN	3.3
1	D	59	GLN	3.3
1	F	32	ILE	3.3
1	D	51	LEU	3.3
1	C	57	ILE	3.2
1	D	61	LYS	3.2
1	F	36	TRP	3.2
1	D	49	GLU	3.2
1	D	74	LYS	3.2
1	F	71	PRO	3.2
1	C	94	VAL	3.2
1	C	62	ALA	3.1
1	B	36	TRP	3.1
1	E	55	GLY	3.1
1	C	61	LYS	3.1
1	A	51	LEU	3.1
1	D	47	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	72	GLY	3.1
1	C	281	ASP	3.1
1	A	52	VAL	3.1
1	D	64	ALA	3.1
1	E	36	TRP	3.1
1	F	70	THR	3.0
1	A	90	GLU	3.0
1	D	4	GLY	3.0
1	D	33	LYS	2.9
1	C	53	ALA	2.9
1	C	49	GLU	2.9
1	F	77	LEU	2.9
1	E	34	GLN	2.9
1	F	57	ILE	2.9
1	F	29	LEU	2.9
1	C	68	ALA	2.8
1	D	94	VAL	2.8
1	D	62	ALA	2.8
1	C	29	LEU	2.8
1	F	73	LEU	2.8
1	D	46	LYS	2.8
1	B	57	ILE	2.8
1	B	26	THR	2.8
1	F	14	GLY	2.8
1	E	74	LYS	2.8
1	B	280	ALA	2.8
1	A	2	LYS	2.8
1	D	65	ILE	2.7
1	C	24	GLY	2.7
1	A	59	GLN	2.7
1	C	72	GLY	2.7
1	D	40	GLY	2.7
1	A	60	GLU	2.7
1	B	33	LYS	2.7
1	A	24	GLY	2.7
1	F	279	ASN	2.6
1	C	58	PRO	2.6
1	D	71	PRO	2.6
1	F	64	ALA	2.6
1	B	32	ILE	2.6
1	F	22	VAL	2.6
1	E	127	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	75	GLU	2.6
1	B	281	ASP	2.6
1	D	91	ASP	2.6
1	F	51	LEU	2.6
1	B	289	GLN	2.6
1	E	89	PHE	2.6
1	C	283	THR	2.6
1	D	72	GLY	2.6
1	F	108	PRO	2.6
1	A	203	GLY	2.6
1	B	255	CYS	2.5
1	C	35	GLU	2.5
1	E	108	PRO	2.5
1	F	58	PRO	2.5
1	F	79	ALA	2.5
1	F	280	ALA	2.5
1	B	77	LEU	2.5
1	D	73	LEU	2.5
1	A	89	PHE	2.5
1	F	65	ILE	2.5
1	E	40	GLY	2.5
1	B	53	ALA	2.4
1	A	71	PRO	2.4
1	F	1	MET	2.4
1	F	15	ILE	2.4
1	C	279	ASN	2.4
1	C	23	GLU	2.4
1	C	102	LEU	2.4
1	D	128	LEU	2.4
1	C	40	GLY	2.4
1	D	90	GLU	2.4
1	A	277	VAL	2.4
1	F	69	ILE	2.4
1	B	22	VAL	2.3
1	F	3	ILE	2.3
1	C	37	ALA	2.3
1	C	48	TYR	2.3
1	B	115	ASN	2.3
1	A	23	GLU	2.3
1	E	282	ARG	2.3
1	F	35	GLU	2.3
1	D	20	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	143	ARG	2.3
1	A	22	VAL	2.3
1	B	94	VAL	2.3
1	C	127	GLY	2.3
1	B	126	LYS	2.2
1	C	73	LEU	2.3
1	C	78	CYS	2.2
1	A	74	LYS	2.2
1	F	129	SER	2.2
1	A	65	ILE	2.2
1	F	61	LYS	2.2
1	F	289	GLN	2.2
1	A	43	LYS	2.2
1	A	45	LYS	2.2
1	B	73	LEU	2.2
1	E	72	GLY	2.2
1	B	71	PRO	2.1
1	D	162	LYS	2.1
1	F	66	VAL	2.1
1	B	72	GLY	2.1
1	D	38	GLU	2.1
1	A	54	LYS	2.1
1	D	39	ASN	2.1
1	C	59	GLN	2.1
1	F	85	VAL	2.1
1	E	110	CYS	2.1
1	E	11	MET	2.1
1	E	73	LEU	2.1
1	E	128	LEU	2.1
1	F	41	LEU	2.1
1	F	50	LYS	2.1
1	F	11	MET	2.1
1	C	51	LEU	2.1
1	F	48	TYR	2.1
1	B	282	ARG	2.1
1	A	20	ALA	2.1
1	E	176	GLN	2.0
1	E	23	GLU	2.0
1	F	60	GLU	2.0
1	B	283	THR	2.0
1	D	26	THR	2.0
1	E	289	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	282	ARG	2.0
1	D	31	ASP	2.0
1	D	37	ALA	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 monosaccharides 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.