



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 AM UTC

PDB ID : 4ASI / pdb_00004asi
Title : Crystal structure of human ACACA C-terminal domain
Authors : Froese, D.S.; Muniz, J.R.C.; Kiyani, W.; Krojer, T.; Vollmar, M.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Oppermann, U.; Yue, W.W.
Deposited on : 2012-05-01
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

<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

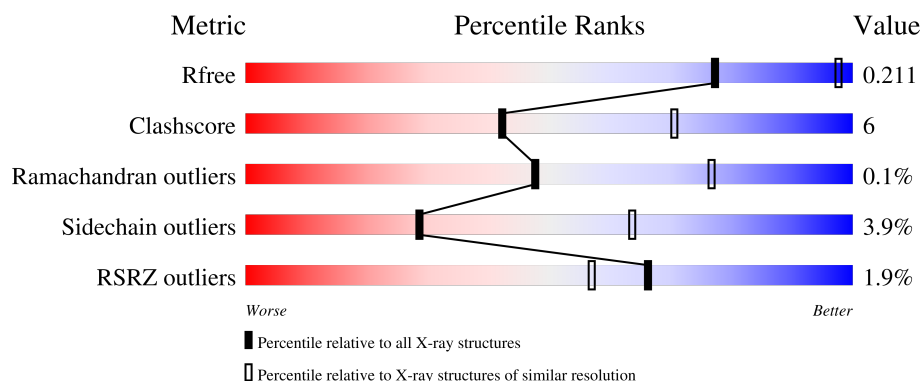
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	769	0.2% 79% 17% ..
1	B	769	0.2% 80% 14% ..
1	C	769	0.2% 80% 17% ..
1	D	769	2% 80% 15% ..
1	E	769	3% 83% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	769	3% 83% 9% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34357 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACETYL-COA CARBOXYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	3	0
			5933	3782	1025	1096	30			
1	B	738	Total	C	N	O	S	0	1	0
			5756	3676	995	1058	27			
1	C	755	Total	C	N	O	S	0	1	0
			5928	3784	1031	1084	29			
1	D	745	Total	C	N	O	S	0	1	0
			5795	3692	1003	1071	29			
1	E	721	Total	C	N	O	S	0	0	0
			5500	3499	957	1019	25			
1	F	718	Total	C	N	O	S	0	1	0
			5416	3443	939	1010	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1607	SER	-	expression tag	UNP Q13085
B	1607	SER	-	expression tag	UNP Q13085
C	1607	SER	-	expression tag	UNP Q13085
D	1607	SER	-	expression tag	UNP Q13085
E	1607	SER	-	expression tag	UNP Q13085
F	1607	SER	-	expression tag	UNP Q13085

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	3	Total	O	0	0
			3	3		
2	C	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	4	Total	O	0	0
			4	4		
2	E	2	Total	O	0	0
			2	2		
2	F	2	Total	O	0	0
			2	2		

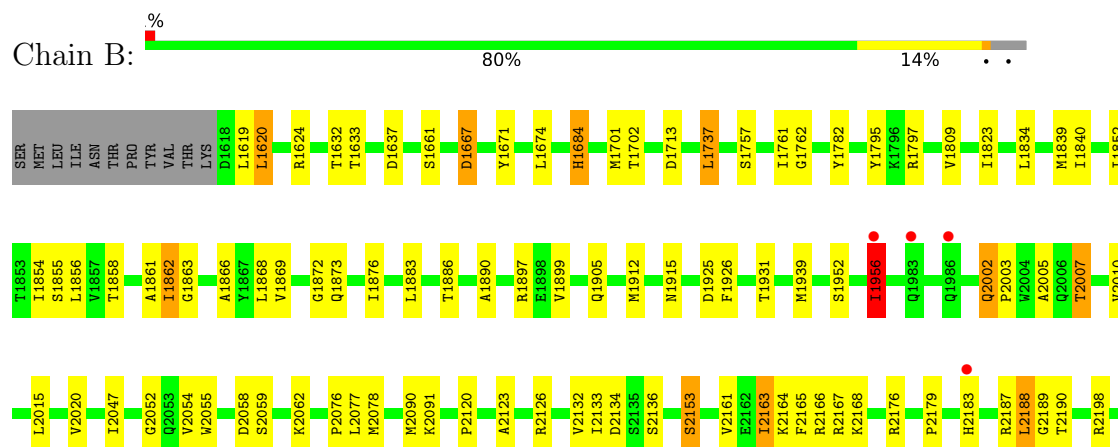
3 Residue-property plots

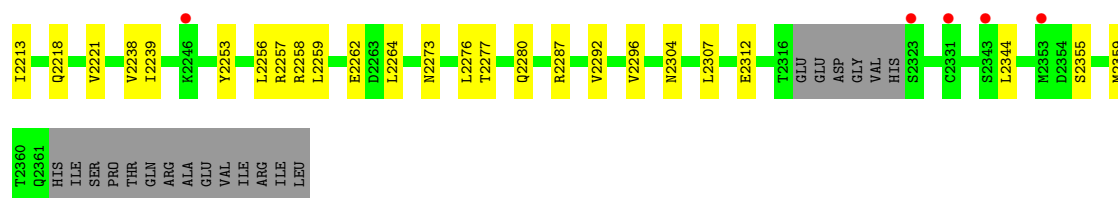
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ACETYL-COA CARBOXYLASE 1

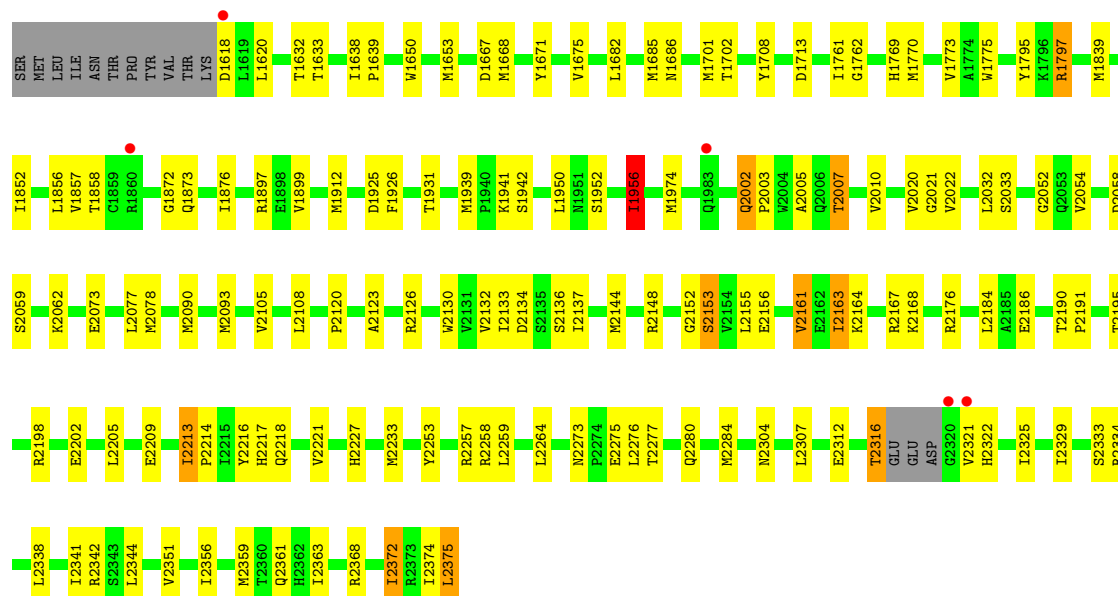
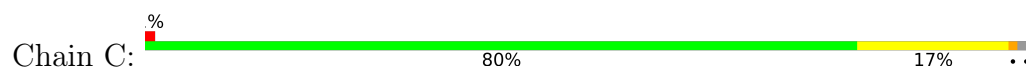


• Molecule 1: ACETYL-COA CARBOXYLASE 1

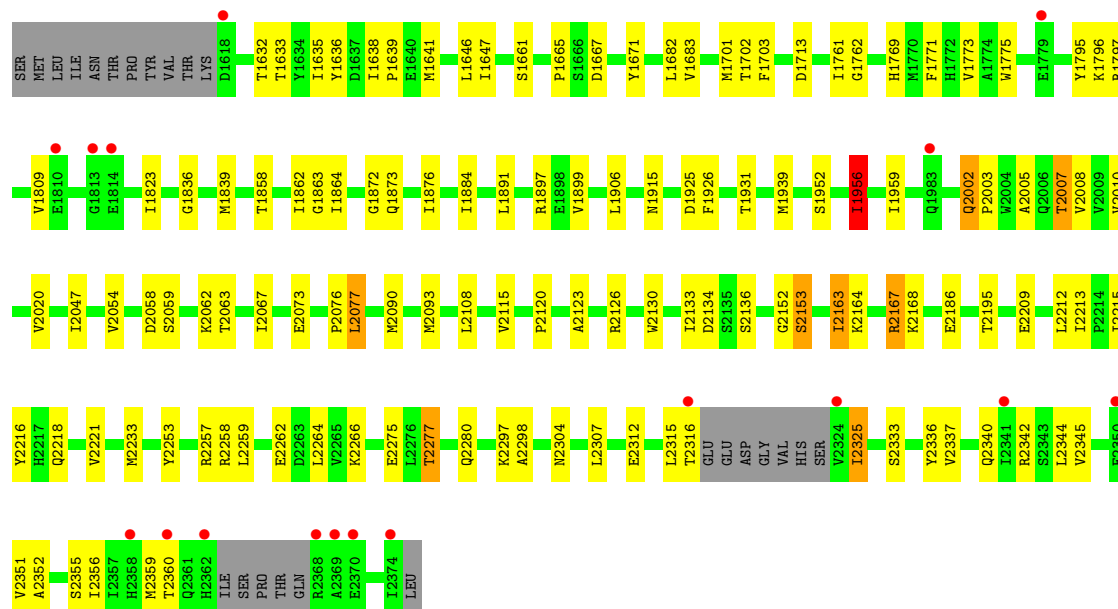
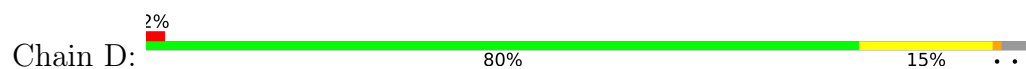




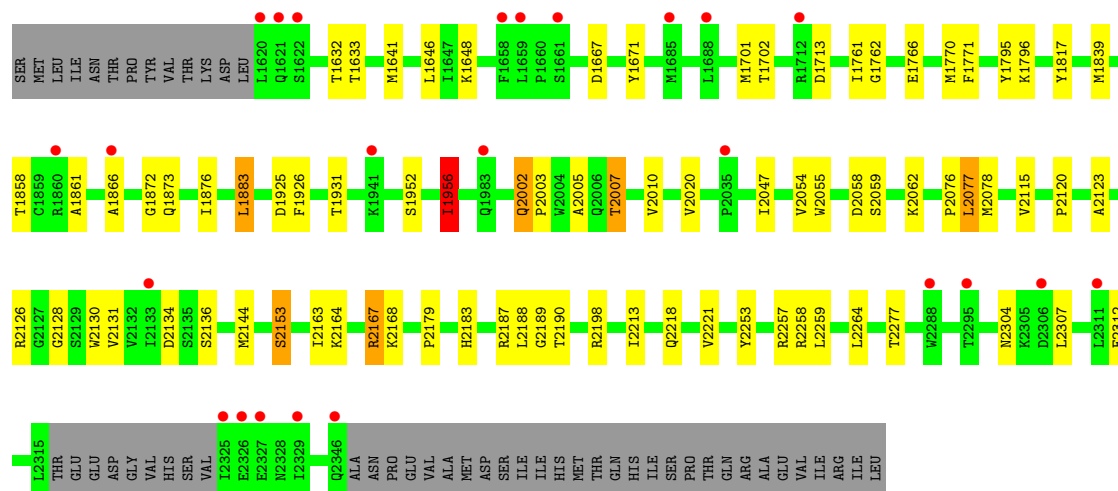
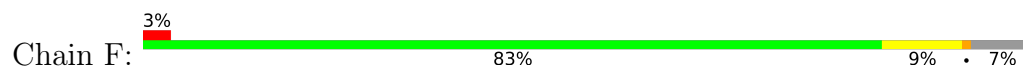
● Molecule 1: ACETYL-COA CARBOXYLASE 1



● Molecule 1: ACETYL-COA CARBOXYLASE 1



Chain E: 3% 83% 10% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.97Å 143.71Å 540.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	540.07 – 2.80 270.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (540.07-2.80) 97.9 (270.04-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.236 (Not available) , 0.211	Depositor DCC
R_{free} test set	10403 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34357	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.45% 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 [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	0.97	3/6081 (0.0%)	1.02	10/8263 (0.1%)
1	B	0.88	1/5897 (0.0%)	0.95	5/8021 (0.1%)
1	C	0.93	5/6071 (0.1%)	1.00	8/8254 (0.1%)
1	D	0.86	1/5933 (0.0%)	0.95	4/8068 (0.0%)
1	E	0.76	0/5632	0.89	2/7668 (0.0%)
1	F	0.75	0/5553	0.88	2/7577 (0.0%)
All	All	0.87	10/35167 (0.0%)	0.95	31/47851 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2161	VAL	CA-CB	8.14	1.64	1.54
1	C	2227	HIS	CG-ND1	-6.37	1.31	1.38
1	C	2217	HIS	N-CA	-6.23	1.38	1.46
1	C	2216	TYR	CA-C	5.77	1.60	1.52
1	A	1919	HIS	CG-CD2	5.57	1.42	1.35
1	C	1769	HIS	CG-CD2	5.51	1.42	1.35
1	A	1882	HIS	CG-ND1	-5.46	1.32	1.38
1	A	1934	HIS	CG-ND1	-5.33	1.32	1.38
1	B	1684	HIS	CG-ND1	-5.14	1.32	1.38
1	D	1769	HIS	CG-CD2	5.13	1.41	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2363	ILE	N-CA-C	7.53	121.00	108.81
1	A	1956	ILE	N-CA-C	-6.52	106.20	111.81
1	A	2368	ARG	N-CA-C	-6.34	104.45	111.36
1	C	2361	GLN	N-CA-C	-6.29	104.53	111.82
1	A	2374	ILE	N-CA-C	6.24	117.36	112.12
1	E	2198	ARG	CG-CD-NE	-6.19	98.38	112.00
1	A	2325	ILE	CB-CA-C	-6.09	104.06	112.04
1	B	2287	ARG	N-CA-CB	5.92	118.92	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2325	ILE	CB-CA-C	-5.88	104.46	111.81
1	B	1956	ILE	N-CA-C	-5.75	106.86	111.81
1	C	2368	ARG	N-CA-C	-5.74	105.10	111.36
1	D	2163	ILE	CB-CA-C	-5.64	104.84	111.94
1	D	1956	ILE	N-CA-C	-5.63	106.97	111.81
1	C	2322	HIS	N-CA-C	-5.58	106.36	112.72
1	A	1638	ILE	CB-CA-C	-5.43	106.89	114.00
1	F	2198	ARG	CG-CD-NE	-5.43	100.06	112.00
1	C	1956	ILE	N-CA-C	-5.38	107.18	111.81
1	B	1862	ILE	CB-CA-C	-5.34	102.66	110.62
1	B	2292	VAL	CB-CA-C	-5.29	105.09	112.02
1	D	2325	ILE	N-CA-C	-5.25	104.85	110.36
1	F	1956	ILE	N-CA-C	-5.23	107.31	111.81
1	C	2161	VAL	N-CA-C	-5.23	105.40	110.42
1	D	2277	THR	CB-CA-C	-5.22	100.28	109.62
1	B	2163	ILE	CB-CA-C	-5.21	105.38	111.94
1	A	1967	THR	CA-C-N	-5.20	114.89	120.03
1	A	1967	THR	C-N-CA	-5.20	114.89	120.03
1	A	2163	ILE	CB-CA-C	-5.16	105.44	111.94
1	C	2148	ARG	CB-CA-C	-5.16	101.91	110.68
1	A	1761	ILE	CB-CA-C	-5.10	102.52	110.69
1	E	1956	ILE	N-CA-C	-5.06	107.46	111.81
1	C	2163	ILE	CB-CA-C	-5.02	105.61	111.94

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	5933	0	5799	97	0
1	B	5756	0	5562	80	0
1	C	5928	0	5775	97	0
1	D	5795	0	5575	81	0
1	E	5500	0	5152	53	0
1	F	5416	0	4973	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	14	0	0	1	0
2	B	3	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
All	All	34357	0	32836	425	0

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 6.

All (425) 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:2167:ARG:NH1	1:C:2209:GLU:OE2	1.75	1.18
1:A:1912:MET:HE1	1:C:2093:MET:HE3	1.31	1.08
1:A:1912:MET:HE1	1:C:2093:MET:CE	1.89	1.01
1:A:1771:PHE:O	1:C:2176:ARG:NH1	2.04	0.90
1:E:2188:LEU:O	1:E:2198:ARG:NH2	2.08	0.86
1:A:2357:ILE:CG1	1:C:2374:ILE:HD13	2.07	0.84
1:C:2276:LEU:HD22	1:C:2284:MET:HE1	1.62	0.81
1:B:2359:MET:HE3	1:D:2345:VAL:HG11	1.65	0.79
1:A:2357:ILE:HG13	1:C:2374:ILE:HD13	1.62	0.79
1:A:2374:ILE:O	1:A:2375:LEU:O	2.00	0.78
1:F:2130:TRP:CE2	1:F:2144:MET:HE1	2.19	0.77
1:A:1737:LEU:CD2	1:A:1839:MET:HE3	2.16	0.75
1:D:1633:THR:HG21	1:D:1641:MET:HE1	1.67	0.75
1:A:1912:MET:CE	1:C:2093:MET:CE	2.65	0.75
1:B:1702:THR:HG23	1:B:1713:ASP:OD1	1.90	0.72
1:C:1632:THR:OG1	1:C:1858:THR:HG21	1.90	0.71
1:D:1939:MET:HE2	1:D:2073:GLU:CD	2.15	0.71
1:D:1632:THR:OG1	1:D:1858:THR:HG21	1.91	0.70
1:B:1912:MET:HE1	1:D:2093:MET:HE3	1.72	0.70
1:D:2007:THR:HG21	1:D:2054:VAL:O	1.91	0.70
1:E:2007:THR:HG21	1:E:2054:VAL:O	1.90	0.70
1:B:2020:VAL:HG12	1:B:2076:PRO:HG2	1.72	0.70
1:E:1939:MET:HE2	1:E:2073:GLU:CD	2.18	0.69
1:D:1665:PRO:HD2	1:E:1686:ASN:O	1.93	0.69
1:A:2020:VAL:HG12	1:A:2076:PRO:HG2	1.75	0.68
1:B:2132:VAL:HG23	1:B:2133:ILE:HG23	1.73	0.68
1:C:2007:THR:HG21	1:C:2054:VAL:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2315:LEU:O	1:D:2316:THR:CB	2.40	0.68
1:C:2312:GLU:O	1:C:2316:THR:HG23	1.93	0.67
1:D:1633:THR:HG21	1:D:1641:MET:CE	2.24	0.67
1:A:2007:THR:HG21	1:A:2054:VAL:O	1.94	0.67
1:A:1737:LEU:HD22	1:A:1839:MET:HE3	1.75	0.66
1:D:2020:VAL:HG12	1:D:2076:PRO:HG2	1.76	0.66
1:A:1886:THR:CG2	1:A:1890:ALA:HB3	2.25	0.66
1:C:1675:VAL:HB	1:C:1685:MET:HE3	1.78	0.66
1:B:1858:THR:HG23	1:B:1925:ASP:OD1	1.95	0.66
1:A:2357:ILE:HG12	1:C:2374:ILE:HD13	1.77	0.65
1:C:2155:LEU:HD12	1:C:2156:GLU:H	1.61	0.64
1:D:2163:ILE:HG22	1:D:2164:LYS:HG2	1.79	0.64
1:F:2007:THR:HG21	1:F:2054:VAL:O	1.96	0.64
1:C:2184:LEU:HB3	1:C:2205:LEU:HD13	1.79	0.64
1:A:2340:GLN:HA	1:A:2340:GLN:OE1	1.98	0.64
1:A:2312:GLU:O	1:A:2316:THR:HG23	1.98	0.63
1:B:1624:ARG:NH1	1:B:1637:ASP:OD1	2.31	0.63
1:F:1795:TYR:CD2	1:F:1817:TYR:CE2	2.87	0.63
1:E:1632:THR:OG1	1:E:1858:THR:HG21	1.98	0.62
1:C:2258:ARG:CZ	1:C:2307:LEU:HD23	2.29	0.62
1:A:1624:ARG:NH1	1:A:1637:ASP:OD1	2.33	0.62
1:F:1858:THR:HG23	1:F:1925:ASP:OD1	1.99	0.62
1:A:1858:THR:HG23	1:A:1925:ASP:OD1	2.00	0.61
1:A:2238:VAL:HG23	1:A:2239:ILE:HG23	1.80	0.61
1:C:2134:ASP:OD2	1:C:2136:SER:HB3	2.01	0.61
1:F:2128:GLY:O	1:F:2131:VAL:HG12	2.00	0.61
1:A:1702:THR:HG23	1:A:1713:ASP:OD1	2.00	0.61
1:B:1912:MET:CE	1:D:2093:MET:HE3	2.30	0.61
1:A:2134:ASP:OD2	1:A:2136:SER:HB3	2.02	0.60
1:B:2007:THR:HG21	1:B:2054:VAL:O	2.01	0.60
1:A:2005:ALA:HB2	1:A:2058:ASP:HB2	1.84	0.59
1:B:2359:MET:HE1	1:D:2355:SER:CB	2.31	0.59
1:C:2163:ILE:HG22	1:C:2164:LYS:HG2	1.85	0.59
1:D:2333:SER:O	1:D:2337:VAL:HG23	2.02	0.59
1:E:1839:MET:HA	1:F:2136:SER:OG	2.01	0.59
1:C:2374:ILE:O	1:C:2375:LEU:HB3	2.02	0.59
1:E:1956:ILE:H	1:E:1956:ILE:HD12	1.67	0.59
1:A:2163:ILE:HG22	1:A:2164:LYS:HG2	1.85	0.59
1:B:1737:LEU:O	1:B:1737:LEU:HD12	2.03	0.59
1:D:2134:ASP:OD2	1:D:2136:SER:HB3	2.03	0.59
1:F:2179:PRO:O	1:F:2183[A]:HIS:ND1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2134:ASP:OD2	1:B:2136:SER:HB3	2.03	0.59
1:D:2108:LEU:HD11	1:D:2133:ILE:HG22	1.85	0.59
1:D:1897:ARG:NH1	1:D:1899:VAL:HG22	2.19	0.58
1:C:1876:ILE:HD13	1:C:1931:THR:HB	1.85	0.58
1:A:1839:MET:HA	1:C:2136:SER:OG	2.04	0.58
1:C:1939:MET:HE2	1:C:2073:GLU:CD	2.29	0.58
1:C:2155:LEU:HD12	1:C:2156:GLU:N	2.19	0.57
1:F:1702:THR:HG23	1:F:1713:ASP:OD1	2.05	0.57
1:A:1905:GLN:O	1:C:2090:MET:HG3	2.03	0.57
1:B:2257:ARG:NH2	1:B:2312:GLU:OE1	2.38	0.57
1:A:2257:ARG:NH2	1:A:2312:GLU:OE1	2.37	0.57
1:A:2351:VAL:HG22	1:C:2338:LEU:HG	1.87	0.57
1:F:2005:ALA:HB2	1:F:2058:ASP:HB2	1.87	0.57
1:A:1632:THR:OG1	1:A:1858:THR:HG21	2.05	0.57
1:D:1876:ILE:HD13	1:D:1931:THR:HB	1.87	0.57
1:B:1897:ARG:NH1	1:B:1899:VAL:HG22	2.20	0.57
1:C:2276:LEU:CD2	1:C:2284:MET:HE1	2.35	0.57
1:E:2134:ASP:OD2	1:E:2136:SER:HB3	2.05	0.57
1:A:2136:SER:OG	1:C:1839:MET:HA	2.05	0.56
1:C:2032:LEU:HD12	1:C:2033:SER:N	2.20	0.56
1:F:1795:TYR:CE2	1:F:1817:TYR:CE2	2.93	0.56
1:F:1956:ILE:HD12	1:F:1956:ILE:H	1.71	0.56
1:F:1632:THR:OG1	1:F:1858:THR:HG21	2.04	0.56
1:B:2179:PRO:O	1:B:2183[B]:HIS:ND1	2.39	0.56
1:E:1897:ARG:NH1	1:E:1899:VAL:HG22	2.20	0.56
1:C:2257:ARG:NH2	1:C:2312:GLU:OE1	2.39	0.56
1:F:2134:ASP:OD2	1:F:2136:SER:HB3	2.04	0.56
1:C:1956:ILE:HD12	1:C:1956:ILE:H	1.70	0.56
1:E:2005:ALA:HB2	1:E:2058:ASP:HB2	1.88	0.56
1:E:2136:SER:OG	1:F:1839:MET:HA	2.05	0.56
1:B:2258:ARG:CZ	1:B:2307:LEU:HD23	2.36	0.55
1:B:2359:MET:HE2	1:D:2352:ALA:HA	1.89	0.55
1:D:2010:VAL:HG22	1:D:2062:LYS:HE3	1.88	0.55
1:E:1858:THR:HG23	1:E:1925:ASP:OD1	2.06	0.55
1:C:2184:LEU:CB	1:C:2205:LEU:HD13	2.36	0.55
1:E:1702:THR:HG23	1:E:1713:ASP:OD1	2.07	0.55
1:E:2257:ARG:NH2	1:E:2312:GLU:OE1	2.39	0.55
1:B:2218:GLN:O	1:B:2221:VAL:HG22	2.07	0.55
1:F:2218:GLN:O	1:F:2221:VAL:HG22	2.06	0.55
1:D:1956:ILE:HD12	1:D:1956:ILE:H	1.73	0.54
1:A:1737:LEU:HD23	1:A:1839:MET:HE3	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2257:ARG:NH2	1:D:2312:GLU:OE1	2.40	0.54
1:B:2005:ALA:HB2	1:B:2058:ASP:HB2	1.88	0.54
1:E:1876:ILE:HD13	1:E:1931:THR:HB	1.90	0.54
1:F:2257:ARG:NH2	1:F:2312:GLU:OE1	2.41	0.54
1:B:1737:LEU:HD12	1:B:1737:LEU:C	2.33	0.54
1:E:2176:ARG:NH1	1:F:1771:PHE:O	2.38	0.54
1:C:1675:VAL:HB	1:C:1685:MET:CE	2.38	0.53
1:F:2187:ARG:C	1:F:2189:GLY:N	2.65	0.53
1:A:1696:MET:HB3	1:A:1735:LEU:HD23	1.89	0.53
1:B:2136:SER:OG	1:D:1839:MET:HA	2.09	0.53
1:C:1897:ARG:NH1	1:C:1899:VAL:HG22	2.24	0.53
1:A:2356:ILE:O	1:A:2360:THR:HG23	2.08	0.52
1:A:2356:ILE:HD11	1:C:2359:MET:HE2	1.90	0.52
1:A:1798:VAL:HA	1:A:1801:LEU:HD12	1.92	0.52
1:B:2187:ARG:C	1:B:2189:GLY:N	2.67	0.52
1:B:2176:ARG:NH1	1:D:1771:PHE:O	2.39	0.52
1:F:2130:TRP:CZ2	1:F:2144:MET:CE	2.92	0.52
1:A:2356:ILE:HG23	1:C:2356:ILE:HD13	1.90	0.52
1:D:2005:ALA:HB2	1:D:2058:ASP:HB2	1.91	0.52
1:D:2167:ARG:HB3	1:D:2167:ARG:HH11	1.75	0.52
1:E:2187:ARG:C	1:E:2189:GLY:N	2.66	0.52
1:B:2163:ILE:HG22	1:B:2164:LYS:HG2	1.92	0.52
1:B:1757:SER:HA	1:B:1862:ILE:HD12	1.91	0.52
1:C:2273:ASN:HB3	1:C:2276:LEU:HD12	1.92	0.51
1:F:1648:LYS:O	1:F:1648:LYS:CD	2.58	0.51
1:B:1632:THR:OG1	1:B:1858:THR:HG21	2.10	0.51
1:B:1839:MET:HA	1:D:2136:SER:OG	2.10	0.51
1:A:1761:ILE:HG22	1:A:1762:GLY:N	2.25	0.51
1:C:1708:TYR:CZ	1:C:1941:LYS:HB3	2.45	0.51
1:E:2163:ILE:HG22	1:E:2164:LYS:HG2	1.92	0.51
1:A:1717:ILE:HG22	1:A:1718:GLY:N	2.25	0.51
1:B:2238:VAL:HG23	1:B:2239:ILE:HG23	1.93	0.51
1:F:2130:TRP:CZ2	1:F:2144:MET:HE2	2.45	0.51
1:E:1708:TYR:CZ	1:E:1941:LYS:HB3	2.46	0.51
1:E:2218:GLN:O	1:E:2221:VAL:HG22	2.10	0.51
1:A:2356:ILE:HD13	1:C:2356:ILE:HG23	1.93	0.50
1:A:1667:ASP:OD2	1:B:1620:LEU:HD23	2.11	0.50
1:F:2258:ARG:CZ	1:F:2307:LEU:HD23	2.42	0.50
1:A:1840:ILE:HG13	1:A:1868:LEU:HD21	1.94	0.50
1:A:2218:GLN:O	1:A:2221:VAL:HG22	2.12	0.50
1:B:1854:ILE:HG22	1:B:1855:SER:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2163:ILE:HG22	1:D:2164:LYS:CG	2.42	0.50
1:D:2167:ARG:NE	1:D:2209:GLU:OE2	2.43	0.50
1:E:2187:ARG:O	1:E:2190:THR:HG23	2.12	0.50
1:A:1632:THR:HB	1:A:1858:THR:HG22	1.93	0.49
1:B:2010:VAL:HG22	1:B:2062:LYS:HE3	1.93	0.49
1:D:2212:LEU:O	1:D:2215:ILE:HG22	2.12	0.49
1:A:2187:ARG:C	1:A:2189:GLY:N	2.67	0.49
1:C:2005:ALA:HB2	1:C:2058:ASP:HB2	1.95	0.49
1:C:1770:MET:HE1	1:C:1797:ARG:NH2	2.28	0.49
1:D:2120:PRO:HD2	1:D:2123:ALA:CB	2.42	0.49
1:F:2130:TRP:CE2	1:F:2144:MET:CE	2.95	0.49
1:A:1696:MET:CG	1:A:1735:LEU:HD23	2.43	0.49
1:A:2273:ASN:HB3	1:A:2276:LEU:HD12	1.95	0.49
1:D:1647:ILE:HG23	1:E:1688:LEU:HD23	1.94	0.49
1:E:1861:ALA:HB3	1:E:1883:LEU:HD13	1.94	0.49
1:E:1646:LEU:HD21	1:E:1703:PHE:HB2	1.95	0.49
1:C:2258:ARG:HG3	1:C:2259:LEU:N	2.28	0.49
1:E:2258:ARG:HD3	1:E:2304:ASN:OD1	2.13	0.49
1:A:1876:ILE:HD13	1:A:1931:THR:HB	1.95	0.48
1:A:2258:ARG:HD3	1:A:2304:ASN:OD1	2.13	0.48
1:B:1876:ILE:HD13	1:B:1931:THR:HB	1.95	0.48
1:E:2120:PRO:HD2	1:E:2123:ALA:CB	2.42	0.48
1:F:2120:PRO:HD2	1:F:2123:ALA:CB	2.43	0.48
1:A:1886:THR:HG23	1:A:1890:ALA:HB3	1.95	0.48
1:B:2020:VAL:HG21	1:B:2078:MET:HE3	1.94	0.48
1:B:2120:PRO:HD2	1:B:2123:ALA:CB	2.42	0.48
1:E:2167:ARG:O	1:E:2168:LYS:C	2.56	0.48
1:A:2258:ARG:CZ	1:A:2307:LEU:HD23	2.43	0.48
1:B:1823:ILE:N	1:B:1823:ILE:HD13	2.29	0.48
1:D:1956:ILE:HG21	1:D:2253:TYR:CD2	2.48	0.48
1:F:1866:ALA:HA	1:F:1883:LEU:HD11	1.96	0.48
1:F:2258:ARG:HD3	1:F:2304:ASN:OD1	2.13	0.48
1:E:1866:ALA:HA	1:E:1883:LEU:HD11	1.95	0.48
1:F:2163:ILE:HG22	1:F:2164:LYS:HG2	1.95	0.48
1:B:1905:GLN:O	1:D:2090:MET:HG3	2.14	0.48
1:D:1891:LEU:HD12	1:D:1906:LEU:HD11	1.95	0.48
1:A:1646:LEU:HD21	1:A:1703:PHE:HB2	1.95	0.48
1:D:2063:THR:O	1:D:2067:ILE:HD12	2.14	0.48
1:F:2002:GLN:HG3	1:F:2003:PRO:HD3	1.95	0.48
1:C:2002:GLN:HG3	1:C:2003:PRO:HD3	1.95	0.48
1:E:2258:ARG:CZ	1:E:2307:LEU:HD23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2010:VAL:HG22	1:F:2062:LYS:HE3	1.96	0.48
1:A:2120:PRO:HD2	1:A:2123:ALA:CB	2.44	0.47
1:B:1632:THR:OG1	1:B:1633:THR:N	2.46	0.47
1:B:2273:ASN:HB3	1:B:2276:LEU:HD12	1.96	0.47
1:C:1632:THR:HB	1:C:1858:THR:HG22	1.94	0.47
1:C:2021:GLY:C	1:C:2022:VAL:HG23	2.39	0.47
1:E:1872:GLY:O	1:E:1873:GLN:HB2	2.14	0.47
1:B:2002:GLN:HG3	1:B:2003:PRO:HD3	1.96	0.47
1:D:2258:ARG:HD3	1:D:2304:ASN:OD1	2.14	0.47
1:C:1632:THR:OG1	1:C:1633:THR:N	2.47	0.47
1:C:2032:LEU:HD12	1:C:2033:SER:H	1.80	0.47
1:C:2184:LEU:HB2	1:C:2205:LEU:CD1	2.45	0.47
1:E:1632:THR:OG1	1:E:1633:THR:N	2.46	0.47
1:E:1956:ILE:HG21	1:E:2253:TYR:CD2	2.49	0.47
1:F:1632:THR:OG1	1:F:1633:THR:N	2.48	0.47
1:F:2007:THR:CG2	1:F:2054:VAL:O	2.63	0.47
1:B:2258:ARG:HD3	1:B:2304:ASN:OD1	2.13	0.47
1:D:2215:ILE:HG23	1:D:2216:TYR:N	2.29	0.47
1:A:1834:LEU:HD13	1:C:2130:TRP:CD2	2.49	0.47
1:D:1632:THR:OG1	1:D:1633:THR:N	2.46	0.47
1:F:2167:ARG:O	1:F:2168:LYS:C	2.57	0.47
1:A:1630:LEU:HD23	1:A:1630:LEU:HA	1.55	0.47
1:B:2052:GLY:O	1:B:2054:VAL:HG23	2.14	0.47
1:C:2105:VAL:HG23	1:C:2132:VAL:HG12	1.95	0.47
1:A:2303:ASN:ND2	1:A:2306:ASP:OD2	2.48	0.47
1:B:1834:LEU:HD13	1:D:2130:TRP:CD2	2.50	0.47
1:B:1956:ILE:HG21	1:B:2253:TYR:CD2	2.50	0.47
1:D:1823:ILE:HD13	1:D:1823:ILE:N	2.30	0.47
1:F:1876:ILE:HD13	1:F:1931:THR:HB	1.97	0.47
1:F:2126:ARG:NH1	1:F:2153:SER:OG	2.48	0.47
1:B:1872:GLY:O	1:B:1873:GLN:HB2	2.14	0.47
1:D:1773:VAL:HG11	1:D:1775:TRP:CE2	2.50	0.47
1:E:2132:VAL:HG23	1:E:2133:ILE:HG23	1.97	0.47
1:F:1761:ILE:HG22	1:F:1762:GLY:N	2.29	0.47
1:B:1862:ILE:HG22	1:B:1863:GLY:N	2.27	0.47
1:B:1840:ILE:HG13	1:B:1868:LEU:HD21	1.97	0.46
1:C:1872:GLY:O	1:C:1873:GLN:HB2	2.15	0.46
1:B:2161:VAL:HG13	1:B:2165:PHE:HB3	1.96	0.46
1:D:1632:THR:HB	1:D:1858:THR:HG22	1.96	0.46
1:F:1872:GLY:O	1:F:1873:GLN:HB2	2.15	0.46
1:A:1761:ILE:CG2	1:A:1762:GLY:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2258:ARG:CZ	1:D:2307:LEU:HD23	2.46	0.46
1:A:2126:ARG:NH1	1:A:2153:SER:OG	2.49	0.46
1:C:1650:TRP:CD1	1:C:1668:MET:HE2	2.50	0.46
1:C:1653:MET:CE	1:C:1950:LEU:HD11	2.45	0.46
1:C:2120:PRO:HD2	1:C:2123:ALA:CB	2.46	0.46
1:B:1886:THR:CG2	1:B:1890:ALA:HB3	2.46	0.46
1:D:1836:GLY:HA2	1:D:1839:MET:HE2	1.97	0.46
1:A:1926:PHE:C	1:A:1926:PHE:CD1	2.94	0.46
1:C:1773:VAL:HG11	1:C:1775:TRP:CE2	2.51	0.46
1:D:2218:GLN:O	1:D:2221:VAL:HG22	2.16	0.46
1:D:2167:ARG:O	1:D:2168:LYS:C	2.59	0.46
1:A:2093:MET:HE3	1:C:1912:MET:CE	2.45	0.46
1:A:2258:ARG:HG3	1:A:2259:LEU:N	2.31	0.46
1:A:2344:LEU:HD12	1:C:2341:ILE:HG13	1.98	0.46
1:B:2355:SER:CB	1:D:2359:MET:HE1	2.46	0.46
1:B:1671:TYR:HB3	1:B:1701:MET:HG2	1.98	0.46
1:B:1956:ILE:HD12	1:B:1956:ILE:H	1.80	0.46
1:B:2126:ARG:NH1	1:B:2153:SER:OG	2.49	0.46
1:A:1632:THR:OG1	1:A:1633:THR:N	2.47	0.46
1:D:1633:THR:CG2	1:D:1641:MET:HE1	2.44	0.46
1:D:1872:GLY:O	1:D:1873:GLN:HB2	2.15	0.46
1:E:2126:ARG:NH1	1:E:2153:SER:OG	2.48	0.46
1:F:1766:GLU:O	1:F:1770:MET:HE3	2.16	0.46
1:F:2179:PRO:C	1:F:2183[A]:HIS:HD1	2.21	0.46
1:B:2167:ARG:O	1:B:2168:LYS:C	2.58	0.45
1:D:1702:THR:HG23	1:D:1713:ASP:OD1	2.16	0.45
1:B:2163:ILE:O	1:B:2166:ARG:NH1	2.47	0.45
1:C:2134:ASP:O	1:C:2137:ILE:HD12	2.16	0.45
1:A:1696:MET:CB	1:A:1735:LEU:HD23	2.45	0.45
1:B:2007:THR:HB	2:B:3001:HOH:O	2.16	0.45
1:C:1761:ILE:HG22	1:C:1762:GLY:N	2.31	0.45
1:C:2273:ASN:HB3	1:C:2276:LEU:CD1	2.47	0.45
1:A:1852:ILE:HD13	1:A:1939:MET:SD	2.57	0.45
1:C:1858:THR:HG23	1:C:1925:ASP:OD1	2.15	0.45
1:C:2167:ARG:O	1:C:2168:LYS:C	2.60	0.45
1:D:2126:ARG:NH1	1:D:2153:SER:OG	2.50	0.45
1:F:2259:LEU:HD23	1:F:2259:LEU:HA	1.75	0.45
1:B:2258:ARG:HG3	1:B:2259:LEU:N	2.31	0.45
1:C:2198:ARG:NE	1:C:2202:GLU:OE2	2.46	0.45
1:A:1757:SER:HA	1:A:1862:ILE:HD12	1.98	0.45
1:C:2258:ARG:HD3	1:C:2304:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2338:LEU:HA	1:C:2338:LEU:HD23	1.74	0.45
1:A:1839:MET:CA	1:C:2136:SER:OG	2.65	0.45
1:C:1956:ILE:HD12	1:C:1956:ILE:N	2.32	0.45
1:C:2078:MET:HE2	1:C:2078:MET:HB3	1.90	0.45
1:E:2163:ILE:O	1:E:2166:ARG:NH1	2.46	0.45
1:A:2167:ARG:O	1:A:2168:LYS:C	2.59	0.45
1:D:2002:GLN:HG3	1:D:2003:PRO:HD3	1.99	0.45
1:D:2008:VAL:HG13	1:D:2062:LYS:HE2	1.98	0.45
1:A:2374:ILE:C	1:A:2375:LEU:O	2.60	0.45
1:B:1674:LEU:HD21	1:B:1684:HIS:CE1	2.51	0.45
1:C:2126:ARG:NH1	1:C:2153:SER:OG	2.50	0.45
1:E:2187:ARG:O	1:E:2190:THR:N	2.49	0.45
1:A:1669:LEU:HD12	1:A:1703:PHE:HB3	1.99	0.44
1:B:2015:LEU:HD22	1:B:2078:MET:HE1	1.98	0.44
1:C:2108:LEU:HD11	1:C:2133:ILE:HG22	1.99	0.44
1:F:1956:ILE:HG21	1:F:2253:TYR:CD2	2.52	0.44
1:B:1854:ILE:CG2	1:B:1855:SER:N	2.80	0.44
1:D:2356:ILE:O	1:D:2360:THR:HG23	2.17	0.44
1:B:1852:ILE:HD13	1:B:1939:MET:SD	2.57	0.44
1:C:1941:LYS:HG2	1:C:1942:SER:N	2.33	0.44
1:C:1671:TYR:HB3	1:C:1701:MET:HG2	2.00	0.44
1:C:2052:GLY:O	1:C:2054:VAL:HG23	2.18	0.44
1:C:2213:ILE:HG22	1:C:2214:PRO:N	2.30	0.44
1:A:1872:GLY:O	1:A:1873:GLN:HB2	2.17	0.44
1:C:1702:THR:HG23	1:C:1713:ASP:OD1	2.17	0.44
1:E:1956:ILE:HD12	1:E:1956:ILE:N	2.31	0.44
1:A:1671:TYR:HB3	1:A:1701:MET:HG2	1.99	0.44
1:A:1956:ILE:HG21	1:A:2253:TYR:CD2	2.52	0.44
1:C:2020:VAL:HG23	1:C:2022:VAL:CG2	2.48	0.44
1:F:1956:ILE:HD12	1:F:1956:ILE:N	2.33	0.44
1:B:2090:MET:HE2	1:B:2091:LYS:HA	2.00	0.44
1:E:2258:ARG:HG3	1:E:2259:LEU:N	2.32	0.44
1:A:2364:SER:OG	1:A:2366:THR:OG1	2.35	0.43
1:D:2007:THR:HB	1:D:2059:SER:OG	2.18	0.43
1:D:2258:ARG:HG3	1:D:2259:LEU:N	2.32	0.43
1:B:2015:LEU:CD2	1:B:2078:MET:HE1	2.48	0.43
1:D:2152:GLY:HA3	1:D:2233:MET:CE	2.48	0.43
1:A:1705:SER:HB2	1:A:1706:PRO:HD2	1.99	0.43
1:E:2167:ARG:HA	1:E:2170:LEU:HD12	2.00	0.43
1:D:1682:LEU:HD12	1:D:1682:LEU:HA	1.79	0.43
1:A:2058:ASP:OD1	1:A:2059:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2187:ARG:O	1:F:2189:GLY:N	2.52	0.43
1:C:2130:TRP:CD1	1:C:2130:TRP:C	2.97	0.43
1:C:2372:ILE:O	1:C:2375:LEU:HD22	2.19	0.43
1:E:1761:ILE:HG22	1:E:1762:GLY:N	2.32	0.43
1:D:1671:TYR:HB3	1:D:1701:MET:HG2	2.01	0.43
1:D:2007:THR:CG2	1:D:2054:VAL:O	2.62	0.43
1:E:1632:THR:HB	1:E:1858:THR:HG22	2.00	0.43
1:F:2258:ARG:HG3	1:F:2259:LEU:N	2.33	0.43
1:A:2364:SER:O	1:A:2367:GLN:N	2.50	0.43
1:C:1856:LEU:HD12	1:C:1857:VAL:N	2.33	0.43
1:E:1926:PHE:CD1	1:E:1926:PHE:C	2.97	0.43
1:A:1912:MET:CE	1:C:2093:MET:HE2	2.46	0.43
1:A:2258:ARG:NH2	1:A:2262:GLU:OE1	2.49	0.43
1:D:1646:LEU:HD21	1:D:1703:PHE:HB2	2.00	0.43
1:D:1858:THR:HG23	1:D:1925:ASP:OD1	2.19	0.43
1:F:2020:VAL:HG12	1:F:2076:PRO:HG2	2.00	0.43
1:B:1926:PHE:CD1	1:B:1926:PHE:C	2.97	0.42
1:B:2007:THR:HB	1:B:2059:SER:OG	2.19	0.42
1:C:2163:ILE:HG22	1:C:2164:LYS:CG	2.48	0.42
1:F:2078:MET:HE2	1:F:2078:MET:HB3	1.85	0.42
1:C:1638:ILE:HB	1:C:1639:PRO:HD3	2.01	0.42
1:D:1926:PHE:CD1	1:D:1926:PHE:C	2.97	0.42
1:E:1839:MET:CA	1:F:2136:SER:OG	2.67	0.42
1:F:1671:TYR:HB3	1:F:1701:MET:HG2	2.00	0.42
1:B:1795:TYR:C	1:B:1797:ARG:H	2.28	0.42
1:B:1915:ASN:OD1	1:B:1915:ASN:C	2.62	0.42
1:D:1915:ASN:OD1	1:D:1915:ASN:C	2.63	0.42
1:A:2007:THR:HB	2:A:3012:HOH:O	2.20	0.42
1:B:1761:ILE:HG22	1:B:1762:GLY:N	2.35	0.42
1:B:2258:ARG:NH2	1:B:2262:GLU:OE1	2.47	0.42
1:C:2258:ARG:CZ	1:C:2307:LEU:CD2	2.97	0.42
1:F:1926:PHE:CD1	1:F:1926:PHE:C	2.97	0.42
1:A:1682:LEU:HD12	1:A:1682:LEU:HA	1.89	0.42
1:A:1915:ASN:C	1:A:1915:ASN:OD1	2.62	0.42
1:D:1773:VAL:HG11	1:D:1775:TRP:CZ2	2.55	0.42
1:D:2262:GLU:HG2	1:D:2266:LYS:HE2	2.02	0.42
1:F:2187:ARG:C	1:F:2189:GLY:H	2.27	0.42
1:B:2188:LEU:O	1:B:2198:ARG:NH2	2.53	0.42
1:D:1635:ILE:HG23	1:D:1636:TYR:N	2.34	0.42
1:A:2187:ARG:O	1:A:2190:THR:N	2.51	0.42
1:B:2058:ASP:OD1	1:B:2059:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1974:MET:HE2	1:C:1974:MET:HB3	1.95	0.42
1:D:1761:ILE:HG22	1:D:1762:GLY:N	2.35	0.42
1:A:2215:ILE:O	1:A:2219:VAL:HG23	2.19	0.41
1:B:2187:ARG:O	1:B:2190:THR:N	2.51	0.41
1:C:1956:ILE:HG21	1:C:2253:TYR:CD2	2.55	0.41
1:C:2010:VAL:HG22	1:C:2062:LYS:HE3	2.02	0.41
1:E:2007:THR:HB	1:E:2059:SER:OG	2.19	0.41
1:A:1674:LEU:C	1:A:1675:VAL:HG23	2.45	0.41
1:B:1862:ILE:CG2	1:B:1863:GLY:N	2.81	0.41
1:B:2078:MET:HE2	1:B:2256:LEU:HD22	2.02	0.41
1:E:1638:ILE:HB	1:E:1639:PRO:HD3	2.02	0.41
1:A:2187:ARG:C	1:A:2189:GLY:H	2.28	0.41
1:D:2297:LYS:O	1:D:2298:ALA:C	2.63	0.41
1:F:1633:THR:HG21	1:F:1641:MET:HE1	2.01	0.41
1:F:2058:ASP:OD1	1:F:2059:SER:N	2.54	0.41
1:A:1620:LEU:HA	1:A:1620:LEU:HD12	1.83	0.41
1:A:1956:ILE:HD12	1:A:1956:ILE:H	1.86	0.41
1:A:2007:THR:HB	1:A:2059:SER:OG	2.20	0.41
1:C:1852:ILE:HD13	1:C:1939:MET:SD	2.61	0.41
1:D:1761:ILE:HD13	1:D:1761:ILE:HG21	1.87	0.41
1:D:1863:GLY:O	1:D:1864:ILE:C	2.63	0.41
1:A:2163:ILE:O	1:A:2166:ARG:NH1	2.47	0.41
1:A:2187:ARG:O	1:A:2189:GLY:N	2.53	0.41
1:C:2184:LEU:CB	1:C:2205:LEU:CD1	2.99	0.41
1:D:1638:ILE:HB	1:D:1639:PRO:HD3	2.02	0.41
1:E:2187:ARG:O	1:E:2189:GLY:N	2.54	0.41
1:A:1697:VAL:HG12	1:A:1698:ALA:N	2.36	0.41
1:B:1866:ALA:HA	1:B:1883:LEU:HD11	2.02	0.41
1:B:2187:ARG:O	1:B:2189:GLY:N	2.53	0.41
1:D:1862:ILE:CD1	1:D:1884:ILE:HG12	2.51	0.41
1:E:1671:TYR:HB3	1:E:1701:MET:HG2	2.02	0.41
1:A:1624:ARG:NH2	1:B:1667:ASP:OD2	2.53	0.41
1:B:1856:LEU:HD13	1:B:1876:ILE:HB	2.03	0.41
1:C:2007:THR:HB	1:C:2059:SER:OG	2.21	0.41
1:C:2152:GLY:HA3	1:C:2233:MET:CE	2.50	0.41
1:D:1862:ILE:HD13	1:D:1884:ILE:HG12	2.01	0.41
1:D:2336:TYR:CE2	1:D:2340:GLN:OE1	2.73	0.41
1:E:2007:THR:CG2	1:E:2054:VAL:O	2.65	0.41
1:A:1773:VAL:HG11	1:A:1775:TRP:CE2	2.55	0.41
1:A:2276:LEU:HD13	1:A:2284:MET:HE1	2.03	0.41
1:B:1861:ALA:HB3	1:B:1883:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1863:GLY:O	1:E:1864:ILE:C	2.63	0.41
1:F:2007:THR:HB	1:F:2059:SER:OG	2.20	0.41
1:F:2054:VAL:HG12	1:F:2055:TRP:N	2.36	0.41
1:A:1708:TYR:CE2	1:A:1948:PRO:HB3	2.56	0.41
1:C:1618:ASP:C	1:C:1620:LEU:N	2.79	0.41
1:C:1926:PHE:CD1	1:C:1926:PHE:C	2.99	0.41
1:C:2007:THR:CG2	1:C:2054:VAL:O	2.66	0.41
1:D:1795:TYR:C	1:D:1797:ARG:H	2.29	0.41
1:B:2187:ARG:C	1:B:2189:GLY:H	2.28	0.40
1:C:1682:LEU:HD12	1:C:1682:LEU:HA	1.85	0.40
1:C:2321:VAL:HG22	1:C:2321:VAL:O	2.21	0.40
1:C:2218:GLN:O	1:C:2221:VAL:HG22	2.21	0.40
1:A:1715:ILE:HD13	1:A:1715:ILE:HA	1.86	0.40
1:A:2002:GLN:N	1:A:2003:PRO:CD	2.85	0.40
1:C:1795:TYR:C	1:C:1797:ARG:H	2.29	0.40
1:D:2002:GLN:N	1:D:2003:PRO:CD	2.84	0.40
1:F:1861:ALA:HB3	1:F:1883:LEU:HD13	2.03	0.40
1:F:2187:ARG:O	1:F:2190:THR:N	2.54	0.40
1:A:1822:ILE:HG21	1:A:1822:ILE:HD13	1.87	0.40
1:C:2190:THR:HA	1:C:2191:PRO:HD3	1.96	0.40
1:D:2058:ASP:OD1	1:D:2059:SER:N	2.54	0.40
1:D:2077:LEU:HB2	1:D:2115:VAL:HG22	2.03	0.40
1:E:1766:GLU:O	1:E:1770:MET:HE3	2.22	0.40
1:E:1941:LYS:HG2	1:E:1942:SER:N	2.35	0.40
1:A:1884:ILE:HG22	1:A:1907:GLY:HA3	2.04	0.40
1:B:1782:TYR:CZ	1:D:2215:ILE:HB	2.56	0.40
1:E:2058:ASP:OD1	1:E:2059:SER:N	2.54	0.40
1:E:2187:ARG:HA	1:E:2190:THR:HG23	2.03	0.40
1:F:2077:LEU:HB2	1:F:2115:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

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	750/769 (98%)	716 (96%)	34 (4%)	0	100	100
1	B	735/769 (96%)	710 (97%)	24 (3%)	1 (0%)	48	77
1	C	752/769 (98%)	722 (96%)	30 (4%)	0	100	100
1	D	740/769 (96%)	712 (96%)	27 (4%)	1 (0%)	48	77
1	E	717/769 (93%)	692 (96%)	23 (3%)	2 (0%)	36	66
1	F	715/769 (93%)	688 (96%)	25 (4%)	2 (0%)	36	66
All	All	4409/4614 (96%)	4240 (96%)	163 (4%)	6 (0%)	48	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2188	LEU
1	E	1796	LYS
1	E	2188	LEU
1	F	2188	LEU
1	D	1796	LYS
1	F	1796	LYS

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	630/672 (94%)	599 (95%)	31 (5%)	22	55
1	B	597/672 (89%)	576 (96%)	21 (4%)	32	67
1	C	620/672 (92%)	592 (96%)	28 (4%)	24	58
1	D	599/672 (89%)	575 (96%)	24 (4%)	28	63
1	E	545/672 (81%)	527 (97%)	18 (3%)	33	69
1	F	525/672 (78%)	511 (97%)	14 (3%)	39	74
All	All	3516/4032 (87%)	3380 (96%)	136 (4%)	28	64

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1618	ASP
1	A	1619	LEU
1	A	1620	LEU
1	A	1661	SER
1	A	1667	ASP
1	A	1683	VAL
1	A	1823	ILE
1	A	1869	VAL
1	A	1947	VAL
1	A	1951	ASN
1	A	1952	SER
1	A	1956	ILE
1	A	2002	GLN
1	A	2007	THR
1	A	2047	ILE
1	A	2055	TRP
1	A	2077	LEU
1	A	2131	VAL
1	A	2153	SER
1	A	2213	ILE
1	A	2238	VAL
1	A	2264	LEU
1	A	2275	GLU
1	A	2277	THR
1	A	2280	GLN
1	A	2334	ARG
1	A	2342	ARG
1	A	2351	VAL
1	A	2356	ILE
1	A	2372	ILE
1	A	2374	ILE
1	B	1619	LEU
1	B	1620	LEU
1	B	1661	SER
1	B	1667	ASP
1	B	1737	LEU
1	B	1809	VAL
1	B	1869	VAL
1	B	1952	SER
1	B	1956	ILE
1	B	2002	GLN
1	B	2007	THR
1	B	2047	ILE

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Mol	Chain	Res	Type
1	B	2055	TRP
1	B	2077	LEU
1	B	2153	SER
1	B	2213	ILE
1	B	2264	LEU
1	B	2277	THR
1	B	2280	GLN
1	B	2296	VAL
1	B	2344	LEU
1	C	1667	ASP
1	C	1686	ASN
1	C	1797	ARG
1	C	1952	SER
1	C	1956	ILE
1	C	2002	GLN
1	C	2007	THR
1	C	2077	LEU
1	C	2144	MET
1	C	2153	SER
1	C	2161	VAL
1	C	2186	GLU
1	C	2195	THR
1	C	2213	ILE
1	C	2264	LEU
1	C	2275	GLU
1	C	2277	THR
1	C	2280	GLN
1	C	2316	THR
1	C	2329	ILE
1	C	2333	SER
1	C	2334	ARG
1	C	2342	ARG
1	C	2344	LEU
1	C	2351	VAL
1	C	2363	ILE
1	C	2372	ILE
1	C	2375	LEU
1	D	1661	SER
1	D	1667	ASP
1	D	1683	VAL
1	D	1809	VAL
1	D	1952	SER

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Mol	Chain	Res	Type
1	D	1956	ILE
1	D	1959	ILE
1	D	2002	GLN
1	D	2007	THR
1	D	2047	ILE
1	D	2077	LEU
1	D	2153	SER
1	D	2167	ARG
1	D	2186	GLU
1	D	2195	THR
1	D	2213	ILE
1	D	2264	LEU
1	D	2275	GLU
1	D	2277	THR
1	D	2280	GLN
1	D	2325	ILE
1	D	2342	ARG
1	D	2344	LEU
1	D	2351	VAL
1	E	1661	SER
1	E	1667	ASP
1	E	1683	VAL
1	E	1802	ASN
1	E	1869	VAL
1	E	1883	LEU
1	E	1952	SER
1	E	1956	ILE
1	E	2007	THR
1	E	2047	ILE
1	E	2077	LEU
1	E	2153	SER
1	E	2161	VAL
1	E	2177	VAL
1	E	2213	ILE
1	E	2264	LEU
1	E	2277	THR
1	E	2280	GLN
1	F	1646	LEU
1	F	1667	ASP
1	F	1883	LEU
1	F	1952	SER
1	F	1956	ILE

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Mol	Chain	Res	Type
1	F	2002	GLN
1	F	2007	THR
1	F	2047	ILE
1	F	2077	LEU
1	F	2153	SER
1	F	2167	ARG
1	F	2213	ILE
1	F	2264	LEU
1	F	2277	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1772	HIS
1	A	1951	ASN
1	A	2071	ASN
1	A	2113	GLN
1	A	2282	GLN
1	A	2314	GLN
1	B	1772	HIS
1	B	1805	HIS
1	B	1944	HIS
1	B	2071	ASN
1	B	2282	GLN
1	B	2314	GLN
1	B	2358	HIS
1	C	1793	GLN
1	C	1802	ASN
1	C	1805	HIS
1	C	1904	ASN
1	C	1919	HIS
1	C	2050	GLN
1	C	2071	ASN
1	C	2282	GLN
1	C	2314	GLN
1	C	2328	ASN
1	D	1772	HIS
1	D	1802	ASN
1	D	2050	GLN
1	D	2282	GLN
1	D	2348	ASN
1	E	1802	ASN

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Mol	Chain	Res	Type
1	E	1805	HIS
1	E	1904	ASN
1	E	1944	HIS
1	E	2053	GLN
1	E	2071	ASN
1	F	1772	HIS
1	F	1802	ASN
1	F	1805	HIS
1	F	1919	HIS
1	F	2050	GLN
1	F	2053	GLN
1	F	2071	ASN
1	F	2282	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 [i](#)

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	751/769 (97%)	-0.46	5 (0%) 84 77	26, 58, 100, 148	3 (0%)
1	B	738/769 (95%)	-0.29	9 (1%) 76 68	35, 72, 123, 161	1 (0%)
1	C	755/769 (98%)	-0.33	5 (0%) 84 77	30, 69, 111, 164	1 (0%)
1	D	745/769 (96%)	-0.23	17 (2%) 61 51	41, 71, 135, 192	1 (0%)
1	E	721/769 (93%)	0.08	26 (3%) 46 37	63, 101, 187, 240	0
1	F	718/769 (93%)	0.20	24 (3%) 49 39	56, 112, 176, 202	1 (0%)
All	All	4428/4614 (95%)	-0.18	86 (1%) 66 57	26, 81, 150, 240	7 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2323	SER	7.0
1	C	2320	GLY	5.8
1	F	2306	ASP	5.3
1	F	1621	GLN	4.9
1	E	2314	GLN	4.8
1	A	2324	VAL	4.6
1	E	2325	ILE	4.4
1	E	1686	ASN	4.3
1	F	2325	ILE	4.3
1	D	1983	GLN	4.1
1	D	1618	ASP	4.1
1	C	1618	ASP	3.7
1	D	1810	GLU	3.7
1	D	2362	HIS	3.6
1	D	2324	VAL	3.5
1	F	2327	GLU	3.5
1	C	1860	ARG	3.4
1	E	1983	GLN	3.4
1	F	1661	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	2346	GLN	3.2
1	D	2374	ILE	3.2
1	E	2298	ALA	3.2
1	E	2327	GLU	3.1
1	E	2315	LEU	2.9
1	B	2343	SER	2.9
1	E	2297	LYS	2.9
1	C	1983	GLN	2.9
1	F	1620	LEU	2.8
1	A	1983	GLN	2.8
1	E	2300	VAL	2.7
1	E	1620	LEU	2.7
1	D	2368	ARG	2.7
1	B	2183[A]	HIS	2.7
1	E	2278	ASP	2.7
1	D	2350	GLU	2.7
1	E	1621	GLN	2.6
1	D	2316	THR	2.6
1	E	2285	LEU	2.6
1	E	2329	ILE	2.6
1	F	2295	THR	2.6
1	E	2265	VAL	2.5
1	C	2321	VAL	2.5
1	F	2326	GLU	2.5
1	F	1658	PHE	2.5
1	B	1983	GLN	2.5
1	F	2288	TRP	2.5
1	F	1688	LEU	2.4
1	F	1983	GLN	2.4
1	A	2375	LEU	2.4
1	D	2341	ILE	2.4
1	E	2304	ASN	2.4
1	F	1685	MET	2.3
1	E	2310	TRP	2.3
1	F	2329	ILE	2.3
1	F	1866	ALA	2.3
1	E	2288	TRP	2.3
1	D	1813	GLY	2.3
1	D	1779	GLU	2.2
1	E	1950	LEU	2.2
1	F	2035	PRO	2.2
1	A	2326	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	2328	ASN	2.2
1	F	1712	ARG	2.2
1	B	2331	CYS	2.2
1	F	2133	ILE	2.2
1	F	1622	SER	2.2
1	F	1941	LYS	2.2
1	F	2311	LEU	2.2
1	D	2370	GLU	2.2
1	D	2360	THR	2.2
1	E	2301	TRP	2.2
1	B	2323	SER	2.2
1	D	2358	HIS	2.1
1	B	2353	MET	2.1
1	D	2369	ALA	2.1
1	A	1914	ASN	2.1
1	E	2087	SER	2.1
1	F	1659	LEU	2.1
1	B	1956	ILE	2.1
1	E	2347	ALA	2.1
1	B	1986	GLN	2.1
1	F	1860	ARG	2.1
1	B	2246	LYS	2.0
1	E	2345	VAL	2.0
1	E	2334	ARG	2.0
1	D	1814	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.