



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:42 PM UTC

PDB ID : 5I6H / pdb_00005i6h
Title : Crystal structure of CD-CT domains of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on : 2016-02-16
Resolution : 7.20 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

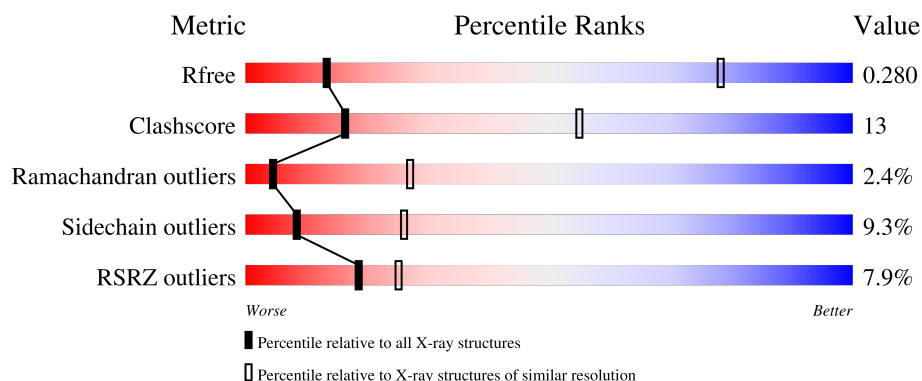
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.20 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	1487	7% 60% 29% 6%
1	B	1487	8% 61% 29% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22543 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.

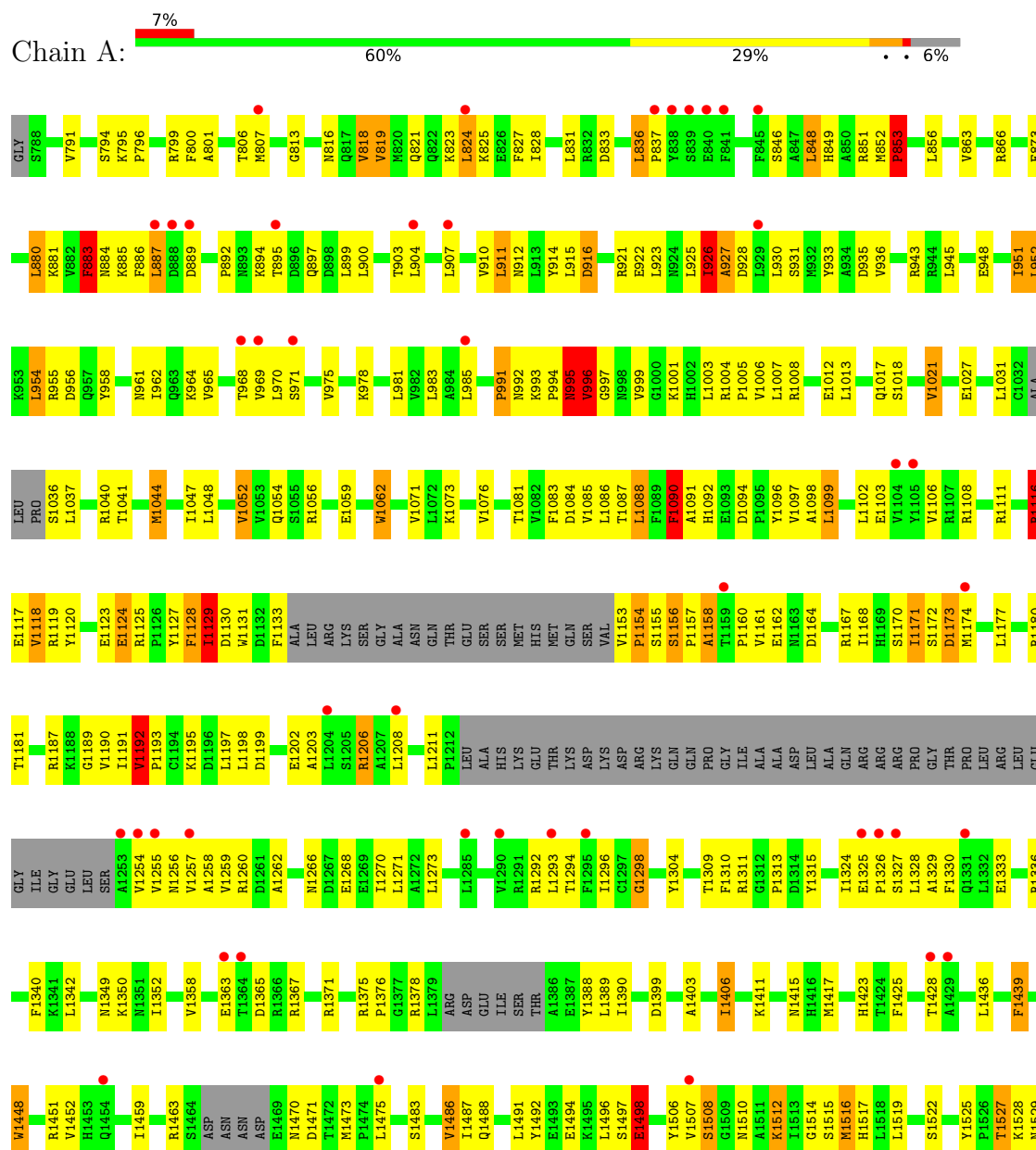
- Molecule 1 is a protein called Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1404	Total	C	N	O	S	0	0	0
			11262	7144	1983	2096	39			
1	B	1406	Total	C	N	O	S	0	0	0
			11281	7156	1988	2098	39			

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-like protein







4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	295.02Å 295.02Å 189.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 7.20 49.85 – 7.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.85-7.20) 99.6 (49.85-7.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 7.37Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.232 , 0.248 0.261 , 0.280	Depositor DCC
R_{free} test set	696 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	662.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 928.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	22543	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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	0.85	7/11439 (0.1%)	1.40	80/15486 (0.5%)
1	B	0.85	6/11458 (0.1%)	1.40	75/15511 (0.5%)
All	All	0.85	13/22897 (0.1%)	1.40	155/30997 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926	ILE	CA-C	8.10	1.63	1.52
1	A	926	ILE	CA-C	7.88	1.62	1.52
1	A	1988	LEU	CA-C	-6.82	1.44	1.52
1	A	2072	ILE	CA-CB	6.33	1.57	1.54
1	B	1988	LEU	CA-C	-6.10	1.45	1.52
1	A	1761	ASP	CA-C	6.06	1.57	1.52
1	B	2072	ILE	CA-CB	5.94	1.57	1.54
1	B	801	ALA	C-N	5.84	1.38	1.33
1	A	801	ALA	C-N	5.53	1.38	1.33
1	A	1864	SER	CA-C	5.47	1.59	1.52
1	B	1864	SER	CA-C	5.40	1.59	1.52
1	A	996	VAL	CA-C	5.06	1.59	1.52
1	B	996	VAL	CA-C	5.03	1.59	1.52

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1261	ASP	CA-CB-CG	9.71	122.31	112.60
1	B	1090	PHE	CA-CB-CG	8.53	122.33	113.80
1	A	1090	PHE	CA-CB-CG	8.13	121.93	113.80
1	B	1980	PHE	CA-CB-CG	8.04	121.84	113.80
1	A	883	PHE	CA-CB-CG	7.76	121.56	113.80
1	B	883	PHE	CA-CB-CG	7.76	121.56	113.80
1	A	1980	PHE	CA-CB-CG	7.75	121.55	113.80
1	A	833	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	819	VAL	CA-C-N	7.59	130.77	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	819	VAL	C-N-CA	7.59	130.77	120.38
1	B	833	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	819	VAL	CA-C-N	7.58	130.76	120.38
1	B	819	VAL	C-N-CA	7.58	130.76	120.38
1	A	853	PRO	CA-C-N	7.39	130.92	120.28
1	A	853	PRO	C-N-CA	7.39	130.92	120.28
1	B	1909	GLU	CB-CG-CD	7.37	125.12	112.60
1	B	853	PRO	CA-C-N	7.34	130.84	120.28
1	B	853	PRO	C-N-CA	7.34	130.84	120.28
1	A	807	MET	CA-C-N	7.27	130.02	120.28
1	A	807	MET	C-N-CA	7.27	130.02	120.28
1	B	1198	LEU	CA-C-N	7.20	130.65	120.28
1	B	1198	LEU	C-N-CA	7.20	130.65	120.28
1	B	1090	PHE	CA-C-N	7.12	132.63	122.09
1	B	1090	PHE	C-N-CA	7.12	132.63	122.09
1	B	807	MET	CA-C-N	7.09	129.78	120.28
1	B	807	MET	C-N-CA	7.09	129.78	120.28
1	B	995	ASN	CA-CB-CG	7.04	119.64	112.60
1	A	1173	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	931	SER	CA-C-N	6.99	129.64	120.28
1	B	931	SER	C-N-CA	6.99	129.64	120.28
1	A	1262	ALA	CA-C-N	6.97	129.95	120.54
1	A	1262	ALA	C-N-CA	6.97	129.95	120.54
1	A	991	PRO	CA-C-N	6.93	132.47	120.68
1	A	991	PRO	C-N-CA	6.93	132.47	120.68
1	A	1090	PHE	CA-C-N	6.93	134.41	122.64
1	A	1090	PHE	C-N-CA	6.93	134.41	122.64
1	B	956	ASP	CA-C-N	6.91	129.54	120.28
1	B	956	ASP	C-N-CA	6.91	129.54	120.28
1	B	991	PRO	CA-C-N	6.90	132.41	120.68
1	B	991	PRO	C-N-CA	6.90	132.41	120.68
1	A	956	ASP	CA-C-N	6.89	129.52	120.28
1	A	956	ASP	C-N-CA	6.89	129.52	120.28
1	A	931	SER	CA-C-N	6.89	129.51	120.28
1	A	931	SER	C-N-CA	6.89	129.51	120.28
1	B	1971	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	1439	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	1439	PHE	CA-CB-CG	6.53	120.33	113.80
1	A	1510	ASN	CA-C-N	6.42	131.25	122.19
1	A	1510	ASN	C-N-CA	6.42	131.25	122.19
1	B	1173	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	1956	GLN	CA-C-N	6.41	130.80	121.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1956	GLN	C-N-CA	6.41	130.80	121.18
1	A	1129	ILE	N-CA-CB	6.35	119.35	111.41
1	A	1971	PHE	CA-CB-CG	6.35	120.15	113.80
1	B	1325	GLU	CB-CG-CD	6.30	123.30	112.60
1	B	1956	GLN	CA-C-N	6.29	130.62	121.18
1	B	1956	GLN	C-N-CA	6.29	130.62	121.18
1	A	873	GLU	CA-C-N	6.24	129.14	120.65
1	A	873	GLU	C-N-CA	6.24	129.14	120.65
1	A	995	ASN	CA-CB-CG	6.24	118.84	112.60
1	B	873	GLU	CA-C-N	6.22	129.11	120.65
1	B	873	GLU	C-N-CA	6.22	129.11	120.65
1	A	1648	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	1422	SER	N-CA-C	-6.20	105.68	113.18
1	B	1741	GLY	CA-C-N	6.19	130.77	120.62
1	B	1741	GLY	C-N-CA	6.19	130.77	120.62
1	A	1999	GLY	CA-C-N	6.17	125.84	119.92
1	A	1999	GLY	C-N-CA	6.17	125.84	119.92
1	B	1648	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	1828	VAL	N-CA-C	-6.11	104.89	110.82
1	B	935	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	925	LEU	CA-C-N	6.06	132.88	121.97
1	B	925	LEU	C-N-CA	6.06	132.88	121.97
1	A	1790	GLU	CB-CG-CD	6.04	122.86	112.60
1	A	925	LEU	CA-C-N	6.03	132.82	121.97
1	A	925	LEU	C-N-CA	6.03	132.82	121.97
1	B	1828	VAL	N-CA-C	-6.01	104.99	110.82
1	B	1826	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	1909	GLU	CB-CG-CD	5.97	122.75	112.60
1	A	1399	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	1741	GLY	CA-C-N	5.94	130.36	120.62
1	A	1741	GLY	C-N-CA	5.94	130.36	120.62
1	A	1826	ASN	CA-CB-CG	5.88	118.48	112.60
1	B	1999	GLY	CA-C-N	5.85	125.54	119.92
1	B	1999	GLY	C-N-CA	5.85	125.54	119.92
1	A	1192	VAL	N-CA-C	5.83	114.55	107.61
1	B	1399	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	2072	ILE	N-CA-CB	5.79	114.40	110.52
1	A	1988	LEU	N-CA-C	5.78	118.96	109.72
1	A	1875	THR	CB-CA-C	5.77	117.21	109.42
1	A	2023	GLU	CB-CG-CD	5.77	122.41	112.60
1	A	1116	ARG	CA-C-N	5.77	132.55	121.54
1	A	1116	ARG	C-N-CA	5.77	132.55	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1118	VAL	N-CA-CB	5.72	117.91	111.21
1	B	1790	GLU	CB-CG-CD	5.68	122.27	112.60
1	B	1875	THR	CB-CA-C	5.63	117.02	109.42
1	B	1510	ASN	CA-CB-CG	5.62	118.22	112.60
1	B	2072	ILE	N-CA-CB	5.62	114.28	110.52
1	A	1298	GLY	N-CA-C	5.61	119.72	110.97
1	A	916	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	1819	GLY	CA-C-N	5.57	127.69	120.44
1	A	1819	GLY	C-N-CA	5.57	127.69	120.44
1	A	927	ALA	CA-C-N	5.57	133.23	122.53
1	A	927	ALA	C-N-CA	5.57	133.23	122.53
1	B	2048	ILE	N-CA-C	-5.57	105.19	110.42
1	A	2048	ILE	N-CA-C	-5.55	105.20	110.42
1	B	927	ALA	CA-C-N	5.55	133.18	122.53
1	B	927	ALA	C-N-CA	5.55	133.18	122.53
1	B	2023	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	1644	LYS	CA-C-N	5.52	127.68	120.28
1	B	1644	LYS	C-N-CA	5.52	127.68	120.28
1	A	935	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	1819	GLY	CA-C-N	5.49	127.57	120.44
1	B	1819	GLY	C-N-CA	5.49	127.57	120.44
1	B	1760	ASN	CA-CB-CG	5.47	118.07	112.60
1	B	916	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	1760	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	928	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	1644	LYS	CA-C-N	5.37	127.47	120.28
1	A	1644	LYS	C-N-CA	5.37	127.47	120.28
1	A	1653	THR	CA-C-N	5.37	127.73	120.38
1	A	1653	THR	C-N-CA	5.37	127.73	120.38
1	A	2007	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	1436	LEU	CA-C-N	5.34	127.70	120.38
1	A	1436	LEU	C-N-CA	5.34	127.70	120.38
1	B	1086	LEU	CA-C-N	5.34	129.23	120.63
1	B	1086	LEU	C-N-CA	5.34	129.23	120.63
1	A	1636	PHE	CA-CB-CG	5.28	119.08	113.80
1	B	1206	ARG	CA-C-N	5.27	127.34	120.28
1	B	1206	ARG	C-N-CA	5.27	127.34	120.28
1	B	928	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	2249	LYS	CA-C-N	5.22	127.23	120.44
1	B	2249	LYS	C-N-CA	5.22	127.23	120.44
1	B	1653	THR	CA-C-N	5.20	127.50	120.38
1	B	1653	THR	C-N-CA	5.20	127.50	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1955	GLU	CA-C-N	-5.17	115.86	123.00
1	B	1955	GLU	C-N-CA	-5.17	115.86	123.00
1	A	1098	ALA	CA-C-N	5.16	127.15	120.44
1	A	1098	ALA	C-N-CA	5.16	127.15	120.44
1	B	2015	ILE	N-CA-C	-5.16	105.68	110.53
1	A	1086	LEU	CA-C-N	5.13	128.89	120.63
1	A	1086	LEU	C-N-CA	5.13	128.89	120.63
1	A	1591	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	1154	PRO	CA-C-N	5.10	131.29	121.54
1	A	1154	PRO	C-N-CA	5.10	131.29	121.54
1	B	2007	GLU	CB-CG-CD	5.09	121.25	112.60
1	B	2174	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	1118	VAL	N-CA-CB	5.07	117.14	111.21
1	B	1091	ALA	CA-C-N	5.04	131.17	121.54
1	B	1091	ALA	C-N-CA	5.04	131.17	121.54
1	A	1206	ARG	CA-C-N	5.02	127.00	120.28
1	A	1206	ARG	C-N-CA	5.02	127.00	120.28
1	B	1636	PHE	CA-CB-CG	5.00	118.81	113.80
1	A	1590	GLY	CA-C-N	5.00	126.94	120.44
1	A	1590	GLY	C-N-CA	5.00	126.94	120.44

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	11262	0	11181	295	0
1	B	11281	0	11205	300	0
All	All	22543	0	22386	582	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 13.

All (582) 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:1389:LEU:HD11	1:B:1425:PHE:HB3	1.33	1.08
1:A:994:PRO:HA	1:A:1037:LEU:HB3	1.35	1.07
1:B:1609:MET:HE1	1:B:1630:VAL:HG13	1.33	1.04
1:B:994:PRO:HA	1:B:1037:LEU:HB3	1.40	1.01
1:A:1090:PHE:HB2	1:A:1193:PRO:HB3	1.39	0.99
1:B:1176:TYR:HE2	1:B:1291:ARG:HD3	1.23	0.98
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.49	0.93
1:A:1125:ARG:HH11	1:A:1203:ALA:HB2	1.31	0.92
1:B:1168:ILE:HB	1:B:1181:THR:HG21	1.51	0.92
1:A:827:PHE:O	1:A:831:LEU:HD23	1.70	0.91
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.51	0.91
1:B:827:PHE:O	1:B:831:LEU:HD23	1.70	0.91
1:A:1192:VAL:HG21	1:A:1203:ALA:HB1	1.53	0.89
1:A:848:LEU:HD23	1:A:851:ARG:HG3	1.55	0.88
1:A:1168:ILE:HB	1:A:1181:THR:HG21	1.57	0.86
1:B:848:LEU:HD23	1:B:851:ARG:HG3	1.54	0.85
1:B:1131:TRP:O	1:B:1188:LYS:HA	1.75	0.85
1:A:852:MET:HB3	1:A:853:PRO:HD2	1.59	0.84
1:A:1376:PRO:HG2	1:A:1423:HIS:HB2	1.57	0.84
1:B:926:ILE:HD12	1:B:985:LEU:HD11	1.59	0.84
1:B:1609:MET:HE1	1:B:1630:VAL:CG1	2.06	0.84
1:B:1059:GLU:HB3	1:B:1062:TRP:HZ3	1.43	0.84
1:B:1176:TYR:CE2	1:B:1291:ARG:HD3	2.11	0.84
1:A:926:ILE:HD12	1:A:985:LEU:HD11	1.60	0.83
1:B:852:MET:HB3	1:B:853:PRO:HD2	1.59	0.83
1:B:1192:VAL:HG11	1:B:1203:ALA:HB1	1.61	0.83
1:A:1980:PHE:HD2	1:A:1988:LEU:HD11	1.43	0.82
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.62	0.81
1:B:1192:VAL:CG1	1:B:1203:ALA:HB1	2.10	0.81
1:A:1059:GLU:HB3	1:A:1062:TRP:HZ3	1.47	0.80
1:B:1127:TYR:HB2	1:B:1193:PRO:HD2	1.64	0.80
1:B:1415:ASN:HB2	1:B:1452:VAL:HA	1.61	0.80
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.64	0.80
1:B:1324:ILE:HG23	1:B:1353:HIS:HE1	1.46	0.79
1:A:1125:ARG:NH1	1:A:1203:ALA:HB2	1.97	0.79
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.63	0.79
1:B:1125:ARG:HD2	1:B:1203:ALA:HB2	1.64	0.79
1:B:1091:ALA:HB2	1:B:1260:ARG:HG2	1.64	0.78
1:B:994:PRO:CA	1:B:1037:LEU:HB3	2.15	0.77
1:B:2249:LYS:HA	1:B:2252:ILE:HD12	1.68	0.76
1:A:1389:LEU:HD13	1:A:1459:ILE:HD11	1.68	0.74
1:A:895:THR:HB	1:A:900:LEU:HD12	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1108:ARG:HH21	1:B:1375:ARG:NH2	1.85	0.74
1:A:1083:PHE:HE2	1:A:1375:ARG:HH12	1.33	0.74
1:B:895:THR:HB	1:B:900:LEU:HD12	1.70	0.74
1:B:961:ASN:O	1:B:965:VAL:HG23	1.87	0.74
1:A:961:ASN:O	1:A:965:VAL:HG23	1.88	0.72
1:B:2037:ARG:HE	1:B:2067:GLU:HA	1.54	0.72
1:B:1516:MET:HG3	1:B:1519:LEU:HD12	1.69	0.72
1:A:1133:PHE:CZ	1:A:1187:ARG:HB2	2.24	0.72
1:B:1090:PHE:HB2	1:B:1193:PRO:HB3	1.72	0.72
1:A:1056:ARG:HD2	1:A:1062:TRP:CZ2	2.25	0.71
1:B:1106:VAL:HG22	1:B:1191:ILE:HD11	1.71	0.70
1:B:1056:ARG:HD2	1:B:1062:TRP:CZ2	2.27	0.70
1:B:1059:GLU:HB3	1:B:1062:TRP:CZ3	2.27	0.70
1:A:1254:VAL:HG11	1:A:1292:ARG:NH2	2.07	0.70
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.72	0.69
1:A:2065:VAL:HG23	1:B:1741:GLY:HA2	1.73	0.69
1:A:1081:THR:HA	1:A:1375:ARG:HH21	1.56	0.68
1:B:1517:HIS:HB3	1:B:1598:VAL:HG23	1.75	0.68
1:B:1336:ARG:HB2	1:B:1371:ARG:NH2	2.07	0.68
1:A:2123:LEU:HD21	1:B:1694:PRO:HG2	1.76	0.68
1:B:1105:TYR:HD2	1:B:1191:ILE:HD13	1.58	0.68
1:A:1127:TYR:HE2	1:A:1190:VAL:HG13	1.59	0.68
1:A:806:THR:HB	1:A:818:VAL:HG11	1.76	0.68
1:B:1336:ARG:HB2	1:B:1371:ARG:HH22	1.59	0.68
1:B:1040:ARG:HH11	1:B:1378:ARG:HG3	1.59	0.67
1:A:1173:ASP:OD1	1:A:1311:ARG:HD3	1.95	0.67
1:B:2241:ASN:HA	1:B:2244:LEU:HD12	1.77	0.67
1:A:1059:GLU:HB3	1:A:1062:TRP:CZ3	2.29	0.66
1:A:1985:GLN:HB3	1:A:2024:LYS:HE3	1.76	0.66
1:A:1515:SER:HA	1:A:1599:SER:O	1.95	0.66
1:A:1486:VAL:C	1:A:1488:GLN:H	2.02	0.66
1:A:2123:LEU:CD2	1:B:1694:PRO:HG2	2.25	0.66
1:A:1448:TRP:HA	1:A:1448:TRP:CE3	2.30	0.66
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.78	0.66
1:B:958:TYR:HB2	1:B:961:ASN:HB2	1.77	0.66
1:B:1173:ASP:OD1	1:B:1311:ARG:HD3	1.97	0.65
1:B:1325:GLU:HB2	1:B:1328:LEU:HB2	1.78	0.65
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.77	0.65
1:B:994:PRO:HA	1:B:1037:LEU:CB	2.21	0.65
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.77	0.65
1:B:1448:TRP:HA	1:B:1448:TRP:CE3	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1490:GLU:OE2	1:B:1514:GLY:HA3	1.96	0.65
1:B:1263:GLU:HG3	1:B:1264:GLY:H	1.62	0.65
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.22	0.64
1:B:1324:ILE:HG23	1:B:1353:HIS:CE1	2.31	0.64
1:B:806:THR:HB	1:B:818:VAL:HG11	1.79	0.64
1:A:958:TYR:HB2	1:A:961:ASN:HB2	1.79	0.64
1:B:1080:TYR:CB	1:B:1378:ARG:HG2	2.28	0.64
1:A:1090:PHE:CB	1:A:1193:PRO:HB3	2.22	0.63
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.81	0.63
1:A:1259:VAL:HG12	1:A:1260:ARG:N	2.14	0.63
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.81	0.63
1:A:936:VAL:HG23	1:A:968:THR:HG23	1.79	0.63
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.81	0.63
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.81	0.63
1:A:853:PRO:HB2	1:A:894:LYS:HD2	1.81	0.63
1:B:856:LEU:HB2	1:B:894:LYS:HE2	1.81	0.63
1:B:853:PRO:HB2	1:B:894:LYS:HD2	1.81	0.62
1:A:936:VAL:HG21	1:A:971:SER:HB3	1.81	0.62
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	1.80	0.62
1:B:1985:GLN:HB3	1:B:2024:LYS:HE3	1.79	0.62
1:B:936:VAL:HG23	1:B:968:THR:HG23	1.81	0.62
1:A:1258:ALA:HA	1:A:1296:ILE:HG23	1.81	0.62
1:A:1054:GLN:HB3	1:A:1062:TRP:CD1	2.35	0.61
1:A:1127:TYR:HB2	1:A:1193:PRO:HD3	1.81	0.61
1:A:1514:GLY:O	1:A:1599:SER:HB3	1.99	0.61
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.82	0.61
1:A:1001:LYS:HA	1:A:1004:ARG:HG3	1.83	0.61
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.40	0.61
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.82	0.61
1:A:856:LEU:HB2	1:A:894:LYS:HE2	1.82	0.61
1:A:927:ALA:HA	1:A:1006:VAL:HG21	1.83	0.61
1:A:1091:ALA:CB	1:A:1260:ARG:HG2	2.31	0.61
1:A:993:LYS:HB2	1:A:994:PRO:HD3	1.82	0.61
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.83	0.61
1:B:936:VAL:HG21	1:B:971:SER:HB3	1.83	0.61
1:B:1001:LYS:HA	1:B:1004:ARG:HG3	1.82	0.61
1:B:1195:LYS:HA	1:B:1260:ARG:HD2	1.83	0.61
1:B:1739:GLY:HA2	1:B:1744:CYS:SG	2.40	0.61
1:B:961:ASN:HA	1:B:964:LYS:HB2	1.83	0.60
1:A:1853:GLN:HG2	1:A:1854:ARG:H	1.65	0.60
1:A:1367:ARG:HH21	1:A:1528:LYS:HG3	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:VAL:HG11	1:B:1017:GLN:HG2	1.82	0.60
1:B:1210:VAL:HG12	1:B:1210:VAL:O	2.02	0.60
1:B:927:ALA:HA	1:B:1006:VAL:HG21	1.84	0.60
1:B:1530:TRP:O	1:B:1533:PRO:HD2	2.00	0.60
1:A:961:ASN:HA	1:A:964:LYS:HB2	1.83	0.60
1:A:1099:LEU:HG	1:A:1120:TYR:CD1	2.37	0.60
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.83	0.60
1:A:975:VAL:HG11	1:A:1017:GLN:HG2	1.83	0.60
1:A:1741:GLY:HA2	1:B:2065:VAL:HG23	1.83	0.59
1:B:1054:GLN:HB3	1:B:1062:TRP:CD1	2.37	0.59
1:B:1187:ARG:HG2	1:B:1291:ARG:HH12	1.66	0.59
1:B:1853:GLN:HG2	1:B:1854:ARG:H	1.66	0.59
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.84	0.59
1:B:1059:GLU:CB	1:B:1062:TRP:HZ3	2.13	0.59
1:B:1389:LEU:HD11	1:B:1425:PHE:CB	2.21	0.59
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.85	0.59
1:A:1127:TYR:CE2	1:A:1190:VAL:HG13	2.36	0.59
1:A:1980:PHE:CD2	1:A:1988:LEU:HD11	2.31	0.59
1:B:1132:ASP:HA	1:B:1187:ARG:O	2.02	0.59
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.84	0.59
1:A:994:PRO:CA	1:A:1037:LEU:HB3	2.22	0.59
1:A:1846:TRP:HZ2	1:A:1910:THR:HG21	1.68	0.59
1:B:856:LEU:CB	1:B:894:LYS:HE2	2.33	0.59
1:A:994:PRO:HA	1:A:1037:LEU:CB	2.24	0.59
1:B:1080:TYR:HB3	1:B:1378:ARG:HG2	1.84	0.58
1:A:1123:GLU:HB2	1:A:1128:PHE:CE1	2.38	0.58
1:B:993:LYS:HB2	1:B:994:PRO:HD3	1.85	0.58
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.84	0.58
1:A:1759:TYR:HB2	1:A:1764:THR:HG21	1.84	0.58
1:A:1195:LYS:HA	1:A:1260:ARG:HD2	1.85	0.58
1:A:1040:ARG:HH22	1:A:1084:ASP:HB3	1.69	0.58
1:B:1292:ARG:NH1	1:B:1326:PRO:HB3	2.19	0.58
1:A:2020:THR:HG21	1:B:1757:ARG:HG2	1.85	0.58
1:B:1426:GLN:HG2	1:B:1462:MET:HB3	1.85	0.58
1:A:1266:ASN:HB3	1:A:1270:ILE:HB	1.86	0.58
1:A:856:LEU:CB	1:A:894:LYS:HE2	2.34	0.58
1:B:1108:ARG:HH21	1:B:1375:ARG:HH22	1.50	0.58
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.86	0.57
1:A:836:LEU:HD12	1:A:914:TYR:OH	2.04	0.57
1:A:1059:GLU:CB	1:A:1062:TRP:HZ3	2.15	0.57
1:A:1091:ALA:HB1	1:A:1260:ARG:HD3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1980:PHE:HD2	1:A:1988:LEU:CD1	2.16	0.57
1:B:2243:LYS:HA	1:B:2246:LYS:HD2	1.87	0.57
1:A:1171:ILE:HD13	1:A:1327:SER:O	2.05	0.57
1:B:852:MET:SD	1:B:903:THR:HG21	2.45	0.57
1:A:1496:LEU:HD12	1:A:1498:GLU:H	1.70	0.56
1:B:877:ARG:HE	1:B:915:LEU:HG	1.69	0.56
1:A:813:GLY:HA3	1:A:971:SER:HA	1.86	0.56
1:A:2253:ALA:HB1	1:A:2257:ARG:HH21	1.70	0.56
1:B:2177:LEU:HA	1:B:2180:ILE:HD12	1.85	0.56
1:A:1340:PHE:CZ	1:A:1527:THR:HG22	2.41	0.56
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.05	0.56
1:A:852:MET:SD	1:A:903:THR:HG21	2.46	0.56
1:A:883:PHE:CE2	1:A:911:LEU:HD21	2.41	0.56
1:A:1497:SER:O	1:A:1498:GLU:HB3	2.05	0.56
1:B:1073:LYS:HA	1:B:1076:VAL:HG22	1.88	0.56
1:B:1844:VAL:HA	1:B:1847:LEU:HD12	1.87	0.56
1:A:948:GLU:O	1:A:952:LEU:HD12	2.06	0.56
1:B:836:LEU:HD12	1:B:914:TYR:OH	2.05	0.55
1:B:1087:THR:HG21	1:B:1298:GLY:HA3	1.88	0.55
1:A:1259:VAL:HG12	1:A:1260:ARG:H	1.71	0.55
1:A:1448:TRP:HA	1:A:1448:TRP:HE3	1.70	0.55
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.71	0.55
1:A:1781:ARG:HH12	1:A:1975:GLN:HE22	1.53	0.55
1:B:1630:VAL:HG11	1:B:1649:PHE:CD2	2.42	0.55
1:B:883:PHE:CE2	1:B:911:LEU:HD21	2.41	0.55
1:B:1448:TRP:HA	1:B:1448:TRP:HE3	1.71	0.55
1:A:795:LYS:HB2	1:A:796:PRO:HD3	1.88	0.55
1:A:1844:VAL:HA	1:A:1847:LEU:HD12	1.89	0.55
1:A:1087:THR:HA	1:A:1090:PHE:CE2	2.42	0.54
1:B:1813:SER:HB3	1:B:1816:GLN:HB2	1.88	0.54
1:B:880:LEU:HD13	1:B:915:LEU:HD12	1.90	0.54
1:B:1195:LYS:CA	1:B:1260:ARG:HD2	2.37	0.54
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.16	0.54
1:B:948:GLU:O	1:B:952:LEU:HD12	2.06	0.54
1:A:1073:LYS:HA	1:A:1076:VAL:HG22	1.89	0.54
1:A:1168:ILE:HB	1:A:1181:THR:CG2	2.35	0.54
1:B:1291:ARG:HG3	1:B:1292:ARG:N	2.23	0.54
1:B:795:LYS:HB2	1:B:796:PRO:HD3	1.88	0.54
1:B:1001:LYS:HG3	1:B:1004:ARG:HH21	1.73	0.54
1:A:1127:TYR:CD2	1:A:1192:VAL:HB	2.43	0.53
1:A:1191:ILE:HG12	1:A:1256:ASN:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.73	0.53
1:A:1846:TRP:CZ2	1:A:1910:THR:HG21	2.43	0.53
1:B:1087:THR:HA	1:B:1090:PHE:CE2	2.43	0.53
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.74	0.53
1:A:1517:HIS:HB3	1:A:1598:VAL:HG23	1.91	0.53
1:A:1813:SER:HB3	1:A:1816:GLN:HB2	1.90	0.53
1:B:887:LEU:HD21	1:B:904:LEU:HD12	1.91	0.53
1:B:945:LEU:HD11	1:B:954:LEU:HD13	1.92	0.52
1:B:1099:LEU:HG	1:B:1120:TYR:CD1	2.44	0.52
1:B:1534:LYS:NZ	1:B:1604:MET:H	2.08	0.52
1:A:1040:ARG:NH2	1:A:1084:ASP:HB3	2.23	0.52
1:A:1091:ALA:HB1	1:A:1260:ARG:CD	2.40	0.52
1:A:1886:TRP:HB3	1:A:1891:LYS:HB2	1.92	0.52
1:A:895:THR:HG23	1:A:895:THR:O	2.09	0.52
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.75	0.52
1:A:1190:VAL:HG12	1:A:1255:VAL:HG23	1.91	0.52
1:A:1001:LYS:HG3	1:A:1004:ARG:HH21	1.75	0.52
1:A:1192:VAL:HG13	1:A:1257:VAL:HG13	1.92	0.52
1:A:1096:TYR:C	1:A:1096:TYR:CD1	2.88	0.52
1:A:1750:LEU:HD13	1:B:2047:THR:HB	1.91	0.52
1:B:2216:TRP:CD1	1:B:2243:LYS:HZ3	2.28	0.52
1:A:1417:MET:HE3	1:A:1452:VAL:HG11	1.91	0.52
1:B:1018:SER:O	1:B:1021:VAL:HG12	2.10	0.52
1:B:1106:VAL:CG2	1:B:1191:ILE:CD1	2.88	0.52
1:A:1885:ARG:HD2	1:A:1919:VAL:HG11	1.90	0.51
1:B:1333:GLU:HG2	1:B:1336:ARG:HG3	1.92	0.51
1:A:948:GLU:OE1	1:A:969:VAL:HG13	2.11	0.51
1:A:1018:SER:O	1:A:1021:VAL:HG12	2.10	0.51
1:A:1088:LEU:O	1:A:1091:ALA:HB3	2.10	0.51
1:B:813:GLY:HA3	1:B:971:SER:HA	1.90	0.51
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	1.92	0.51
1:B:852:MET:HB2	1:B:900:LEU:HD21	1.92	0.51
1:B:1109:ALA:O	1:B:1327:SER:HB2	2.10	0.51
1:A:2181:GLU:OE1	1:A:2181:GLU:HA	2.07	0.51
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.92	0.51
1:A:1638:ILE:HD12	1:A:1640:SER:HB3	1.91	0.51
1:B:831:LEU:HD12	1:B:922:GLU:HA	1.92	0.51
1:B:1106:VAL:CG2	1:B:1191:ILE:HD11	2.37	0.51
1:A:887:LEU:HD21	1:A:904:LEU:HD12	1.92	0.51
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.90	0.51
1:B:895:THR:HG23	1:B:895:THR:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:GLU:OE1	1:B:969:VAL:HG13	2.10	0.51
1:B:996:VAL:HG22	1:B:1036:SER:N	2.25	0.51
1:B:1125:ARG:HH21	1:B:1202:GLU:HB2	1.76	0.51
1:B:1417:MET:HE3	1:B:1452:VAL:HG11	1.93	0.51
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.93	0.51
1:A:1048:LEU:O	1:A:1052:VAL:HG23	2.11	0.51
1:A:1127:TYR:HB2	1:A:1193:PRO:CD	2.40	0.51
1:B:1168:ILE:HD12	1:B:1181:THR:OG1	2.10	0.51
1:A:831:LEU:HD12	1:A:922:GLU:HA	1.93	0.51
1:A:1928:ILE:HD11	1:A:2168:ARG:HG3	1.93	0.51
1:B:1154:PRO:HB2	1:B:1158:ALA:HB2	1.92	0.51
1:B:2037:ARG:HH11	1:B:2068:PRO:HD3	1.75	0.51
1:A:1811:TYR:CE1	1:B:2001:GLN:HB2	2.46	0.51
1:B:1096:TYR:CD1	1:B:1096:TYR:C	2.89	0.51
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.76	0.51
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.93	0.51
1:B:2022:PHE:HE2	1:B:2024:LYS:HB2	1.75	0.51
1:B:2143:ARG:HH12	1:B:2147:LYS:HE2	1.74	0.51
1:B:1047:ILE:HG23	1:B:1071:VAL:HG12	1.93	0.50
1:A:1403:ALA:O	1:A:1406:ILE:HG13	2.12	0.50
1:B:1332:LEU:HG	1:B:1371:ARG:HB3	1.92	0.50
1:A:1389:LEU:HD13	1:A:1459:ILE:CD1	2.40	0.50
1:A:852:MET:HB2	1:A:900:LEU:HD21	1.93	0.50
1:B:1048:LEU:O	1:B:1052:VAL:HG23	2.11	0.50
1:B:1187:ARG:HG2	1:B:1291:ARG:HH22	1.77	0.50
1:A:1091:ALA:HB1	1:A:1260:ARG:HG2	1.94	0.50
1:A:1102:LEU:O	1:A:1106:VAL:HG23	2.12	0.50
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.18	0.50
1:B:1027:GLU:O	1:B:1031:LEU:HG	2.12	0.50
1:A:1304:TYR:HB3	1:A:1350:LYS:HB2	1.94	0.50
1:A:2137:LEU:HA	1:A:2140:ARG:HD3	1.94	0.50
1:B:886:PHE:HB3	1:B:894:LYS:HG2	1.94	0.50
1:B:1081:THR:HG23	1:B:1375:ARG:HE	1.77	0.50
1:A:2022:PHE:HE2	1:A:2024:LYS:HB2	1.75	0.50
1:B:1340:PHE:CZ	1:B:1527:THR:HG22	2.47	0.50
1:A:1103:GLU:OE1	1:A:1118:VAL:HG21	2.12	0.50
1:B:1885:ARG:HD2	1:B:1919:VAL:HG11	1.93	0.50
1:A:1534:LYS:NZ	1:A:1604:MET:H	2.09	0.49
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.94	0.49
1:A:1047:ILE:HG23	1:A:1071:VAL:HG12	1.95	0.49
1:A:1378:ARG:HB2	1:A:1388:TYR:CZ	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:LEU:O	1:B:911:LEU:HD13	2.12	0.49
1:B:1702:TYR:HA	1:B:1729:LYS:HA	1.94	0.49
1:A:852:MET:HB3	1:A:853:PRO:CD	2.38	0.49
1:A:1759:TYR:CE2	1:A:1784:GLN:HG3	2.47	0.49
1:A:2047:THR:HB	1:B:1750:LEU:HD13	1.93	0.49
1:B:823:LYS:NZ	1:B:981:LEU:HD11	2.27	0.49
1:A:1197:LEU:HD13	1:A:1273:LEU:HD23	1.94	0.49
1:B:897:GLN:HB3	1:B:899:LEU:CD2	2.42	0.49
1:B:1403:ALA:O	1:B:1406:ILE:HG13	2.11	0.49
1:A:995:ASN:HB2	1:A:999:VAL:HG22	1.94	0.49
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.12	0.49
1:B:824:LEU:O	1:B:828:ILE:HG12	2.12	0.49
1:B:994:PRO:HB3	1:B:1037:LEU:HD22	1.94	0.49
1:A:824:LEU:O	1:A:828:ILE:HG12	2.12	0.49
1:A:1702:TYR:HA	1:A:1729:LYS:HA	1.95	0.49
1:A:1259:VAL:CG1	1:A:1260:ARG:H	2.25	0.49
1:A:886:PHE:HB3	1:A:894:LYS:HG2	1.94	0.49
1:A:897:GLN:HB3	1:A:899:LEU:CD2	2.43	0.49
1:A:1171:ILE:HG22	1:A:1329:ALA:HB3	1.95	0.49
1:A:1757:ARG:HG2	1:B:2020:THR:HG21	1.94	0.49
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.94	0.49
1:A:2143:ARG:HH12	1:A:2147:LYS:HE2	1.78	0.49
1:B:995:ASN:HB2	1:B:999:VAL:HG22	1.95	0.49
1:A:923:LEU:HD21	1:A:999:VAL:HG12	1.94	0.49
1:A:1171:ILE:HG23	1:A:1330:PHE:N	2.27	0.49
1:A:1259:VAL:CG1	1:A:1260:ARG:N	2.76	0.49
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.95	0.49
1:A:2169:ARG:O	1:A:2173:GLU:HB2	2.13	0.49
1:B:880:LEU:HG	1:B:911:LEU:HD23	1.95	0.49
1:B:1127:TYR:HE2	1:B:1190:VAL:CG1	2.26	0.49
1:A:1119:ARG:HB2	1:A:1130:ASP:HB3	1.94	0.49
1:B:1527:THR:O	1:B:1530:TRP:HD1	1.96	0.49
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.13	0.49
1:A:907:LEU:O	1:A:911:LEU:HD13	2.13	0.48
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.94	0.48
1:A:2028:ILE:HB	1:A:2055:MET:HG3	1.94	0.48
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	1.94	0.48
1:A:1056:ARG:HD2	1:A:1062:TRP:HZ2	1.76	0.48
1:B:2072:ILE:CG2	1:B:2073:PRO:HD3	2.42	0.48
1:A:1164:ASP:H	1:A:1167:ARG:NE	2.11	0.48
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:PRO:HB2	1:A:1158:ALA:HB2	1.94	0.48
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.96	0.48
1:B:887:LEU:HD22	1:B:900:LEU:HB3	1.96	0.48
1:B:1164:ASP:H	1:B:1167:ARG:NE	2.11	0.48
1:B:2028:ILE:HB	1:B:2055:MET:HG3	1.94	0.48
1:B:881:LYS:HA	1:B:884:ASN:OD1	2.14	0.48
1:A:887:LEU:HD22	1:A:900:LEU:HB3	1.95	0.48
1:B:933:TYR:HD1	1:B:978:LYS:HG2	1.79	0.48
1:B:1424:THR:HA	1:B:1460:ASN:HB2	1.95	0.48
1:B:2143:ARG:NH1	1:B:2147:LYS:HE2	2.27	0.48
1:A:837:PRO:HB3	1:A:914:TYR:CD1	2.49	0.48
1:B:1127:TYR:HE2	1:B:1190:VAL:HG13	1.76	0.48
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.79	0.48
1:B:1479:ILE:HA	1:B:1488:GLN:O	2.14	0.48
1:B:1638:ILE:HD12	1:B:1640:SER:HB3	1.95	0.48
1:A:994:PRO:HB3	1:A:1037:LEU:HD22	1.96	0.48
1:A:1358:VAL:HA	1:A:1365:ASP:O	2.13	0.48
1:B:1044:MET:HE3	1:B:1085:VAL:HG13	1.96	0.48
1:B:1462:MET:SD	1:B:1469:GLU:HB3	2.54	0.48
1:A:823:LYS:NZ	1:A:981:LEU:HD11	2.29	0.47
1:B:1333:GLU:O	1:B:1334:LEU:HB2	2.14	0.47
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.96	0.47
1:A:1091:ALA:HB2	1:A:1260:ARG:HG2	1.95	0.47
1:B:1307:TYR:CZ	1:B:1325:GLU:HG3	2.49	0.47
1:A:800:PHE:HB2	1:A:836:LEU:HD21	1.97	0.47
1:A:1325:GLU:C	1:A:1327:SER:H	2.22	0.47
1:B:887:LEU:HD22	1:B:900:LEU:HD13	1.96	0.47
1:A:881:LYS:HA	1:A:884:ASN:OD1	2.13	0.47
1:A:933:TYR:HD1	1:A:978:LYS:HG2	1.79	0.47
1:B:1091:ALA:CB	1:B:1260:ARG:HG2	2.39	0.47
1:B:1481:ASN:HA	1:B:1486:VAL:HA	1.95	0.47
1:A:880:LEU:HG	1:A:911:LEU:HD23	1.95	0.47
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	1.97	0.47
1:A:2177:LEU:HA	1:A:2180:ILE:HD12	1.96	0.47
1:B:1054:GLN:HB3	1:B:1062:TRP:NE1	2.30	0.47
1:B:1162:GLU:HG3	1:B:1522:SER:OG	2.14	0.47
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.97	0.47
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.97	0.47
1:B:837:PRO:HB3	1:B:914:TYR:CD1	2.49	0.47
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.95	0.47
1:B:1477:VAL:HG23	1:B:1490:GLU:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:LEU:HD11	1:A:969:VAL:HG21	1.96	0.47
1:A:1621:TYR:OH	1:A:1851:PRO:HA	2.15	0.47
1:B:952:LEU:HD11	1:B:969:VAL:HG21	1.96	0.47
1:B:1928:ILE:HD11	1:B:2168:ARG:HG3	1.95	0.47
1:A:887:LEU:HD22	1:A:900:LEU:HD13	1.97	0.47
1:A:936:VAL:HG23	1:A:968:THR:CG2	2.44	0.47
1:A:1129:ILE:HD11	1:A:1191:ILE:HB	1.97	0.47
1:B:1492:TYR:HA	1:B:1506:TYR:HA	1.97	0.47
1:A:991:PRO:C	1:A:994:PRO:HD2	2.40	0.47
1:A:1336:ARG:HB3	1:A:1525:TYR:CE2	2.49	0.47
1:B:895:THR:CB	1:B:900:LEU:HD12	2.43	0.47
1:B:1292:ARG:CZ	1:B:1326:PRO:HB3	2.45	0.47
1:B:1790:GLU:HA	1:B:1820:THR:HG21	1.96	0.47
1:B:885:LYS:O	1:B:889:ASP:HB3	2.15	0.46
1:B:1114:ASN:O	1:B:1133:PHE:HD1	1.98	0.46
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.96	0.46
1:B:1102:LEU:O	1:B:1106:VAL:HG23	2.15	0.46
1:B:1344:PRO:HA	1:B:1355:TYR:HA	1.96	0.46
1:A:996:VAL:HG22	1:A:1036:SER:N	2.31	0.46
1:A:1054:GLN:HB3	1:A:1062:TRP:NE1	2.30	0.46
1:A:945:LEU:HD11	1:A:954:LEU:HD13	1.97	0.46
1:A:1160:PRO:HG2	1:A:1494:GLU:OE2	2.16	0.46
1:B:948:GLU:O	1:B:951:ILE:HG22	2.16	0.46
1:A:2143:ARG:NH1	1:A:2147:LYS:HE2	2.30	0.46
1:A:885:LYS:O	1:A:889:ASP:HB3	2.15	0.46
1:A:955:ARG:HH22	1:A:968:THR:HG21	1.81	0.46
1:A:2116:MET:C	1:A:2118:GLN:H	2.24	0.46
1:B:2070:GLY:O	1:B:2073:PRO:HD2	2.15	0.46
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.97	0.46
1:A:2241:ASN:HA	1:A:2244:LEU:HD12	1.96	0.46
1:B:1040:ARG:NH2	1:B:1084:ASP:HB3	2.30	0.46
1:B:1091:ALA:HB1	1:B:1260:ARG:HD3	1.98	0.46
1:A:863:VAL:O	1:A:866:ARG:HG2	2.16	0.46
1:A:2249:LYS:HA	1:A:2252:ILE:HD12	1.97	0.46
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.97	0.46
1:B:2057:ALA:HB3	1:B:2150:ILE:HD13	1.98	0.46
1:A:1125:ARG:HD2	1:A:1203:ALA:HB2	1.98	0.46
1:B:1621:TYR:OH	1:B:1851:PRO:HA	2.16	0.46
1:A:1915:ALA:HB2	1:A:1968:ASN:HB2	1.98	0.45
1:A:1935:VAL:HB	1:A:1993:ASN:HB3	1.98	0.45
1:B:863:VAL:O	1:B:866:ARG:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1863:PRO:HB2	1:B:1867:PRO:HA	1.98	0.45
1:A:948:GLU:O	1:A:951:ILE:HG22	2.16	0.45
1:A:1631:ALA:HB2	1:A:1666:LEU:HB2	1.99	0.45
1:B:836:LEU:HG	1:B:921:ARG:HH12	1.81	0.45
1:B:1125:ARG:CD	1:B:1203:ALA:HB2	2.41	0.45
1:B:1668:ALA:HB2	1:B:1769:THR:HG23	1.98	0.45
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.98	0.45
1:B:910:VAL:O	1:B:914:TYR:HD2	1.99	0.45
1:B:1884:VAL:HG21	1:B:1935:VAL:O	2.16	0.45
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.97	0.45
1:A:1044:MET:HE3	1:A:1085:VAL:HG13	1.99	0.45
1:A:1131:TRP:CE3	1:A:1189:GLY:HA3	2.51	0.45
1:A:1293:LEU:O	1:A:1309:THR:HA	2.15	0.45
1:B:1354:VAL:HG22	1:B:1370:THR:HG23	1.99	0.45
1:A:1367:ARG:NH2	1:A:1528:LYS:HG3	2.29	0.45
1:A:2057:ALA:HB3	1:A:2150:ILE:HD13	1.99	0.45
1:A:2256:MET:HA	1:A:2259:LEU:HD12	1.98	0.45
1:B:1935:VAL:HB	1:B:1993:ASN:HB3	1.98	0.45
1:A:2070:GLY:O	1:A:2073:PRO:HD2	2.16	0.45
1:B:923:LEU:HD21	1:B:999:VAL:HG12	1.98	0.45
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.98	0.45
1:A:1790:GLU:HA	1:A:1820:THR:HG21	1.98	0.45
1:B:800:PHE:HB2	1:B:836:LEU:HD21	1.98	0.45
1:B:1480:THR:H	1:B:1488:GLN:HB3	1.82	0.45
1:B:1631:ALA:HB2	1:B:1666:LEU:HB2	1.99	0.45
1:B:955:ARG:HH22	1:B:968:THR:HG21	1.82	0.45
1:B:1965:TRP:HB3	1:B:1997:PHE:CE2	2.52	0.45
1:B:2005:TYR:C	1:B:2007:GLU:H	2.25	0.45
1:A:1162:GLU:HG3	1:A:1522:SER:HB3	1.98	0.45
1:A:1516:MET:HG3	1:A:1519:LEU:HD22	1.98	0.45
1:B:1080:TYR:HB2	1:B:1378:ARG:HG2	1.99	0.45
1:A:846:SER:HA	1:A:849:HIS:ND1	2.32	0.44
1:A:910:VAL:O	1:A:914:TYR:HD2	2.00	0.44
1:A:1161:VAL:HG22	1:A:1162:GLU:H	1.82	0.44
1:B:846:SER:HA	1:B:849:HIS:ND1	2.32	0.44
1:B:1630:VAL:HG12	1:B:1665:TYR:HD1	1.83	0.44
1:B:1094:ASP:HB3	1:B:1097:VAL:HG23	1.99	0.44
1:B:1108:ARG:O	1:B:1111:ARG:HG3	2.17	0.44
1:B:1640:SER:OG	1:B:1673:ARG:HG2	2.17	0.44
1:A:852:MET:O	1:A:853:PRO:C	2.60	0.44
1:A:2072:ILE:CG2	1:A:2073:PRO:HD3	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.99	0.44
1:B:2116:MET:C	1:B:2118:GLN:H	2.25	0.44
1:A:836:LEU:HG	1:A:921:ARG:HH12	1.82	0.44
1:A:1161:VAL:HG22	1:A:1162:GLU:N	2.33	0.44
1:A:1191:ILE:HA	1:A:1256:ASN:O	2.18	0.44
1:A:1486:VAL:C	1:A:1488:GLN:N	2.74	0.44
1:B:852:MET:O	1:B:853:PRO:C	2.61	0.44
1:B:1477:VAL:HG22	1:B:1479:ILE:HD11	1.99	0.44
1:A:1908:VAL:HG23	1:A:1908:VAL:O	2.17	0.44
1:A:1096:TYR:O	1:A:1099:LEU:HB3	2.17	0.44
1:A:1108:ARG:O	1:A:1111:ARG:HG3	2.17	0.44
1:A:1676:LEU:HG	1:B:2138:HIS:CE1	2.53	0.44
1:B:1194:CYS:SG	1:B:1203:ALA:CB	3.06	0.44
1:A:1052:VAL:HG22	1:A:1096:TYR:CE1	2.53	0.44
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	2.00	0.44
1:B:1333:GLU:HB2	1:B:1371:ARG:NH1	2.33	0.44
1:B:1609:MET:CE	1:B:1630:VAL:HG13	2.25	0.44
1:A:1005:PRO:HA	1:A:1008:ARG:HG2	2.00	0.43
1:A:1195:LYS:HA	1:A:1260:ARG:CD	2.48	0.43
1:A:1965:TRP:HB3	1:A:1997:PHE:CE2	2.53	0.43
1:B:1416:HIS:HD2	1:B:1454:GLN:HG3	1.83	0.43
1:A:951:ILE:O	1:A:955:ARG:HG3	2.18	0.43
1:A:1390:ILE:HB	1:A:1439:PHE:HE2	1.83	0.43
1:A:1884:VAL:HG21	1:A:1935:VAL:O	2.17	0.43
1:B:1423:HIS:HE1	1:B:1425:PHE:HD1	1.66	0.43
1:B:2047:THR:HA	1:B:2050:PRO:HG3	2.00	0.43
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	2.01	0.43
1:A:2046:PRO:HA	1:A:2053:MET:SD	2.59	0.43
1:B:1915:ALA:HB2	1:B:1968:ASN:HB2	1.99	0.43
1:B:1324:ILE:CG2	1:B:1353:HIS:HE1	2.24	0.43
1:B:1369:PHE:CD2	1:B:1416:HIS:HB3	2.54	0.43
1:A:1668:ALA:HB2	1:A:1769:THR:HG23	2.00	0.43
1:A:1741:GLY:CA	1:B:2065:VAL:HG23	2.47	0.43
1:B:1527:THR:O	1:B:1530:TRP:CD1	2.72	0.43
1:A:1640:SER:OG	1:A:1673:ARG:HG2	2.18	0.43
1:B:1742:VAL:HA	1:B:1745:LEU:HD12	2.01	0.43
1:A:895:THR:CB	1:A:900:LEU:HD12	2.43	0.43
1:A:1094:ASP:HB3	1:A:1097:VAL:HG23	2.00	0.43
1:A:1371:ARG:HH22	1:A:1525:TYR:HE2	1.65	0.43
1:B:1005:PRO:HA	1:B:1008:ARG:HG2	2.00	0.43
1:B:1737:GLU:HG2	1:B:1740:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:SER:HB2	1:A:1173:ASP:HB2	2.01	0.43
1:B:1588:VAL:HG21	1:B:1600:ARG:NH1	2.34	0.43
1:A:883:PHE:HE2	1:A:911:LEU:HD21	1.83	0.43
1:A:1336:ARG:HB3	1:A:1525:TYR:CD2	2.54	0.43
1:A:1663:ARG:HH21	1:A:1765:CYS:H	1.66	0.43
1:B:969:VAL:HG12	1:B:973:LYS:HE3	2.01	0.43
1:A:1127:TYR:CD2	1:A:1127:TYR:C	2.96	0.42
1:A:1863:PRO:HB2	1:A:1867:PRO:HA	2.01	0.42
1:B:2077:LYS:H	1:B:2080:LYS:HD2	1.84	0.42
1:B:936:VAL:HG23	1:B:968:THR:CG2	2.45	0.42
1:B:1052:VAL:HG22	1:B:1096:TYR:CE1	2.54	0.42
1:A:2047:THR:HA	1:A:2050:PRO:HG3	2.00	0.42
1:A:2065:VAL:HG23	1:B:1741:GLY:CA	2.44	0.42
1:B:1106:VAL:HG11	1:B:1131:TRP:CD1	2.53	0.42
1:A:1776:GLY:O	1:A:1780:VAL:HG23	2.19	0.42
1:A:1781:ARG:NH1	1:A:1975:GLN:HE22	2.15	0.42
1:A:2134:PHE:HA	1:A:2137:LEU:HD12	2.02	0.42
1:B:1506:TYR:CE1	1:B:1517:HIS:HB2	2.54	0.42
1:A:2029:TYR:HA	1:A:2056:TYR:O	2.20	0.42
1:A:2032:PRO:O	1:A:2033:HIS:HB3	2.19	0.42
1:B:1461:CYS:O	1:B:1461:CYS:SG	2.78	0.42
1:B:1480:THR:O	1:B:1486:VAL:HG13	2.18	0.42
1:B:810:ILE:HG21	1:B:981:LEU:HD23	2.01	0.42
1:B:883:PHE:HE2	1:B:911:LEU:HD21	1.83	0.42
1:B:951:ILE:O	1:B:955:ARG:HG3	2.19	0.42
1:B:1096:TYR:O	1:B:1099:LEU:HB3	2.19	0.42
1:B:1106:VAL:HG23	1:B:1191:ILE:HD12	2.02	0.42
1:B:2032:PRO:O	1:B:2033:HIS:HB3	2.19	0.42
1:A:791:VAL:HB	1:A:794:SER:HB3	2.01	0.42
1:A:1389:LEU:HD11	1:A:1425:PHE:CB	2.50	0.42
1:B:837:PRO:HB3	1:B:914:TYR:CE1	2.55	0.42
1:B:994:PRO:HA	1:B:1037:LEU:H	1.83	0.42
1:A:1123:GLU:HB3	1:A:1124:GLU:H	1.73	0.42
1:A:1358:VAL:CG1	1:A:1363:GLU:HA	2.50	0.42
1:A:1717:THR:HB	1:A:1728:HIS:HB3	2.02	0.42
1:A:1742:VAL:HA	1:A:1745:LEU:HD12	2.01	0.42
1:B:1319:ASP:O	1:B:1344:PRO:HG2	2.20	0.42
1:A:852:MET:CB	1:A:853:PRO:HD2	2.42	0.41
1:A:837:PRO:HB3	1:A:914:TYR:CE1	2.55	0.41
1:A:1909:GLU:HG2	1:A:1910:THR:N	2.34	0.41
1:A:2005:TYR:C	1:A:2007:GLU:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1390:ILE:HB	1:B:1439:PHE:HE2	1.84	0.41
1:B:1842:LYS:O	1:B:1845:GLN:HB3	2.20	0.41
1:B:2134:PHE:HA	1:B:2137:LEU:HD12	2.01	0.41
1:B:1099:LEU:O	1:B:1099:LEU:HD23	2.20	0.41
1:B:1776:GLY:O	1:B:1780:VAL:HG23	2.19	0.41
1:A:1087:THR:CB	1:A:1298:GLY:HA3	2.50	0.41
1:B:1113:TYR:HA	1:B:1153:VAL:HG22	2.02	0.41
1:A:1087:THR:HB	1:A:1298:GLY:HA3	2.02	0.41
1:A:1535:ARG:HA	1:A:1545:TYR:HB2	2.03	0.41
1:A:2214:GLU:HG2	1:A:2222:PHE:CD1	2.56	0.41
1:B:1784:GLN:HE22	1:B:1975:GLN:NE2	2.19	0.41
1:B:2046:PRO:HA	1:B:2053:MET:SD	2.60	0.41
1:A:821:GLN:O	1:A:825:LYS:HG2	2.21	0.41
1:B:821:GLN:O	1:B:825:LYS:HG2	2.20	0.41
1:B:1106:VAL:HG22	1:B:1191:ILE:CD1	2.43	0.41
1:B:1535:ARG:HA	1:B:1545:TYR:HB2	2.03	0.41
1:B:1659:MET:HB2	1:B:1661:ILE:HG12	2.03	0.41
1:A:1125:ARG:HD2	1:A:1203:ALA:HA	2.02	0.41
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.84	0.41
1:B:2256:MET:HE2	1:B:2256:MET:HB3	2.00	0.41
1:A:2138:HIS:CE1	1:B:1676:LEU:HG	2.57	0.40
1:B:1717:THR:HB	1:B:1728:HIS:HB3	2.02	0.40
1:B:1858:LEU:HD12	1:B:2171:LEU:HD21	2.03	0.40
1:B:2029:TYR:HA	1:B:2056:TYR:O	2.20	0.40
1:A:800:PHE:CB	1:A:836:LEU:HD21	2.51	0.40
1:A:1208:LEU:HD23	1:A:1211:LEU:HD12	2.02	0.40
1:A:1588:VAL:HG21	1:A:1600:ARG:NH1	2.36	0.40
1:A:1842:LYS:O	1:A:1845:GLN:HB3	2.21	0.40
1:A:2019:LEU:HB3	1:A:2053:MET:CE	2.52	0.40
1:A:2109:SER:HA	1:A:2112:ILE:HD12	2.03	0.40
1:B:791:VAL:HB	1:B:794:SER:HB3	2.02	0.40
1:B:1988:LEU:HD22	1:B:1990:ILE:CD1	2.50	0.40
1:A:1629:VAL:HG22	1:A:1664:ILE:HB	2.04	0.40
1:A:1737:GLU:HG2	1:A:1740:LEU:HD21	2.03	0.40
1:A:2184:ILE:HD12	1:A:2209:HIS:CE1	2.56	0.40
1:B:1056:ARG:HD2	1:B:1062:TRP:HZ2	1.78	0.40
1:B:1197:LEU:HD13	1:B:1273:LEU:HD23	2.03	0.40
1:B:1473:MET:HE3	1:B:1475:LEU:HD21	2.04	0.40
1:B:1908:VAL:O	1:B:1908:VAL:HG23	2.20	0.40
1:B:2109:SER:HA	1:B:2112:ILE:HD12	2.02	0.40
1:B:2217:VAL:HG12	1:B:2219:ILE:H	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:LEU:HD13	1:A:985:LEU:HD23	2.03	0.40
1:A:1156:SER:HB2	1:A:1157:PRO:HD3	2.03	0.40
1:A:1294:THR:OG1	1:A:1326:PRO:HG3	2.21	0.40
1:B:1160:PRO:HA	1:B:1502:TRP:CD1	2.57	0.40
1:B:1898:GLN:H	1:B:1898:GLN:HG2	1.80	0.40
1:A:1794:ILE:HD12	1:A:1823:MET:HG3	2.04	0.40
1:B:921:ARG:HE	1:B:921:ARG:HB3	1.78	0.40

There are no symmetry-related clashes.

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	1378/1487 (93%)	1221 (89%)	121 (9%)	36 (3%)	4	25
1	B	1380/1487 (93%)	1221 (88%)	130 (9%)	29 (2%)	5	30
All	All	2758/2974 (93%)	2442 (88%)	251 (9%)	65 (2%)	4	27

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	VAL
1	A	943	ARG
1	A	1092	HIS
1	A	1117	GLU
1	A	1128	PHE
1	A	1156	SER
1	A	1487	ILE
1	A	1784	GLN
1	A	1864	SER
1	B	819	VAL
1	B	943	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1128	PHE
1	B	1156	SER
1	B	1864	SER
1	A	853	PRO
1	A	1486	VAL
1	A	2038	GLY
1	A	2201	ALA
1	A	2225	ASN
1	B	853	PRO
1	B	997	GLY
1	B	1486	VAL
1	B	2038	GLY
1	B	2201	ALA
1	B	2225	ASN
1	A	892	PRO
1	A	997	GLY
1	A	1158	ALA
1	A	1572	ALA
1	B	892	PRO
1	B	1092	HIS
1	B	1155	SER
1	B	1180	ARG
1	A	887	LEU
1	A	1116	ARG
1	A	1155	SER
1	A	1180	ARG
1	A	1333	GLU
1	A	1516	MET
1	A	1570	SER
1	A	1638	ILE
1	B	887	LEU
1	B	1570	SER
1	B	1572	ALA
1	B	1638	ILE
1	B	1784	GLN
1	B	1790	GLU
1	A	1313	PRO
1	A	1498	GLU
1	A	1508	SER
1	A	1512	LYS
1	A	1527	THR
1	A	1576	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1790	GLU
1	B	1158	ALA
1	B	1313	PRO
1	B	1487	ILE
1	B	1576	PRO
1	B	1516	MET
1	A	1052	VAL
1	B	1052	VAL
1	A	926	ILE
1	B	926	ILE
1	B	996	VAL
1	A	996	VAL

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	1213/1282 (95%)	1099 (91%)	114 (9%)	8	25
1	B	1215/1282 (95%)	1104 (91%)	111 (9%)	9	27
All	All	2428/2564 (95%)	2203 (91%)	225 (9%)	8	26

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	799	ARG
1	A	816	ASN
1	A	818	VAL
1	A	824	LEU
1	A	836	LEU
1	A	848	LEU
1	A	880	LEU
1	A	883	PHE
1	A	911	LEU
1	A	912	ASN
1	A	915	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	916	ASP
1	A	951	ILE
1	A	952	LEU
1	A	954	LEU
1	A	962	ILE
1	A	970	LEU
1	A	983	LEU
1	A	992	ASN
1	A	995	ASN
1	A	1003	LEU
1	A	1007	LEU
1	A	1012	GLU
1	A	1013	LEU
1	A	1021	VAL
1	A	1041	THR
1	A	1044	MET
1	A	1062	TRP
1	A	1088	LEU
1	A	1090	PHE
1	A	1099	LEU
1	A	1116	ARG
1	A	1124	GLU
1	A	1129	ILE
1	A	1153	VAL
1	A	1171	ILE
1	A	1172	SER
1	A	1174	MET
1	A	1177	LEU
1	A	1192	VAL
1	A	1198	LEU
1	A	1199	ASP
1	A	1324	ILE
1	A	1328	LEU
1	A	1342	LEU
1	A	1406	ILE
1	A	1411	LYS
1	A	1428	THR
1	A	1448	TRP
1	A	1463	ARG
1	A	1470	ASN
1	A	1471	ASP
1	A	1473	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1475	LEU
1	A	1483	SER
1	A	1498	GLU
1	A	1507	VAL
1	A	1529	ASN
1	A	1557	ILE
1	A	1563	GLU
1	A	1567	LYS
1	A	1570	SER
1	A	1571	LEU
1	A	1574	LYS
1	A	1593	ASP
1	A	1595	LEU
1	A	1599	SER
1	A	1604	MET
1	A	1632	ASN
1	A	1638	ILE
1	A	1652	CYS
1	A	1659	MET
1	A	1663	ARG
1	A	1674	LEU
1	A	1676	LEU
1	A	1715	VAL
1	A	1729	LYS
1	A	1730	ILE
1	A	1731	ILE
1	A	1760	ASN
1	A	1762	ILE
1	A	1764	THR
1	A	1771	ARG
1	A	1773	VAL
1	A	1775	ILE
1	A	1815	LEU
1	A	1817	LEU
1	A	1885	ARG
1	A	1898	GLN
1	A	1901	LEU
1	A	1917	THR
1	A	1940	ILE
1	A	1941	GLU
1	A	1942	ASN
1	A	1957	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1958	THR
1	A	1965	TRP
1	A	1968	ASN
1	A	1975	GLN
1	A	1988	LEU
1	A	2007	GLU
1	A	2009	LEU
1	A	2023	GLU
1	A	2076	TYR
1	A	2078	LYS
1	A	2088	LEU
1	A	2166	ARG
1	A	2168	ARG
1	A	2171	LEU
1	A	2175	ASP
1	A	2181	GLU
1	A	2197	THR
1	A	2240	ILE
1	A	2247	LEU
1	B	799	ARG
1	B	816	ASN
1	B	818	VAL
1	B	824	LEU
1	B	836	LEU
1	B	848	LEU
1	B	880	LEU
1	B	883	PHE
1	B	911	LEU
1	B	912	ASN
1	B	915	LEU
1	B	916	ASP
1	B	944	ARG
1	B	951	ILE
1	B	952	LEU
1	B	954	LEU
1	B	962	ILE
1	B	970	LEU
1	B	983	LEU
1	B	992	ASN
1	B	995	ASN
1	B	1003	LEU
1	B	1007	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1012	GLU
1	B	1013	LEU
1	B	1021	VAL
1	B	1041	THR
1	B	1044	MET
1	B	1088	LEU
1	B	1090	PHE
1	B	1099	LEU
1	B	1118	VAL
1	B	1124	GLU
1	B	1127	TYR
1	B	1130	ASP
1	B	1171	ILE
1	B	1172	SER
1	B	1174	MET
1	B	1177	LEU
1	B	1192	VAL
1	B	1198	LEU
1	B	1332	LEU
1	B	1333	GLU
1	B	1334	LEU
1	B	1379	LEU
1	B	1406	ILE
1	B	1422	SER
1	B	1432	VAL
1	B	1434	GLU
1	B	1448	TRP
1	B	1469	GLU
1	B	1483	SER
1	B	1489	ILE
1	B	1496	LEU
1	B	1507	VAL
1	B	1513	ILE
1	B	1557	ILE
1	B	1563	GLU
1	B	1567	LYS
1	B	1570	SER
1	B	1571	LEU
1	B	1574	LYS
1	B	1593	ASP
1	B	1595	LEU
1	B	1599	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1604	MET
1	B	1630	VAL
1	B	1638	ILE
1	B	1652	CYS
1	B	1659	MET
1	B	1674	LEU
1	B	1676	LEU
1	B	1715	VAL
1	B	1729	LYS
1	B	1730	ILE
1	B	1731	ILE
1	B	1760	ASN
1	B	1762	ILE
1	B	1771	ARG
1	B	1773	VAL
1	B	1775	ILE
1	B	1815	LEU
1	B	1817	LEU
1	B	1885	ARG
1	B	1898	GLN
1	B	1901	LEU
1	B	1909	GLU
1	B	1917	THR
1	B	1940	ILE
1	B	1941	GLU
1	B	1942	ASN
1	B	1957	VAL
1	B	1958	THR
1	B	1965	TRP
1	B	1968	ASN
1	B	1975	GLN
1	B	1988	LEU
1	B	2007	GLU
1	B	2009	LEU
1	B	2023	GLU
1	B	2076	TYR
1	B	2078	LYS
1	B	2088	LEU
1	B	2166	ARG
1	B	2168	ARG
1	B	2171	LEU
1	B	2175	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2197	THR
1	B	2256	MET
1	B	2258	GLU
1	B	2260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	995	ASN
1	A	1323	HIS
1	A	1410	ASN
1	A	1453	HIS
1	A	1529	ASN
1	A	1555	GLN
1	A	1558	GLN
1	A	1950	ASN
1	A	1956	GLN
1	A	1975	GLN
1	A	1978	ASN
1	A	1985	GLN
1	A	2049	ASN
1	A	2129	GLN
1	A	2133	GLN
1	A	2196	ASN
1	A	2212	GLN
1	B	1043	GLN
1	B	1331	GLN
1	B	1410	ASN
1	B	1416	HIS
1	B	1453	HIS
1	B	1555	GLN
1	B	1558	GLN
1	B	1898	GLN
1	B	1950	ASN
1	B	1978	ASN
1	B	1985	GLN
1	B	2049	ASN
1	B	2129	GLN
1	B	2133	GLN
1	B	2196	ASN
1	B	2212	GLN
1	B	2255	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2261:ARG	C	2300:UNK	N	9.73

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	1392/1487 (93%)	0.21	106 (7%)	20 26	33, 251, 497, 500	0
1	B	1394/1487 (93%)	0.23	115 (8%)	17 25	13, 262, 498, 500	0
All	All	2786/2974 (93%)	0.22	221 (7%)	18 25	13, 258, 497, 500	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	933	TYR	14.2
1	A	2256	MET	10.8
1	B	2256	MET	9.9
1	A	2092	TYR	8.4
1	A	2088	LEU	8.4
1	B	1684	PHE	8.4
1	A	1684	PHE	8.3
1	B	929	LEU	7.9
1	A	1680	LEU	7.8
1	B	2006	ASN	7.7
1	A	1730	ILE	7.3
1	A	1701	LEU	7.2
1	A	2259	LEU	7.2
1	B	973	LYS	6.9
1	B	2233	TYR	6.8
1	B	1525	TYR	6.8
1	B	824	LEU	6.7
1	A	1290	VAL	6.6
1	A	2099	MET	6.2
1	B	932	MET	6.2
1	B	930	LEU	6.1
1	B	1686	VAL	6.1
1	A	841	PHE	6.1
1	A	1429	ALA	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2176	ILE	5.9
1	B	2092	TYR	5.9
1	A	1253	ALA	5.8
1	A	2213	LEU	5.7
1	B	1701	LEU	5.5
1	B	811	LEU	5.4
1	B	2119	ARG	5.3
1	A	2089	ASP	5.3
1	B	939	GLN	5.3
1	B	942	GLY	5.3
1	A	1715	VAL	5.2
1	A	2006	ASN	5.2
1	B	807	MET	5.2
1	B	937	GLU	5.2
1	B	948	GLU	5.1
1	A	1255	VAL	5.0
1	B	1888	ILE	5.0
1	B	2134	PHE	5.0
1	B	951	ILE	4.9
1	B	2259	LEU	4.9
1	A	807	MET	4.9
1	B	936	VAL	4.8
1	B	1293	LEU	4.8
1	B	2120	GLU	4.8
1	B	2085	MET	4.8
1	B	1680	LEU	4.7
1	A	1285	LEU	4.6
1	B	968	THR	4.6
1	A	2039	GLY	4.6
1	A	2085	MET	4.5
1	B	2123	LEU	4.4
1	B	883	PHE	4.4
1	A	1204	LEU	4.4
1	B	1944	THR	4.3
1	B	2213	LEU	4.3
1	B	1010	LEU	4.3
1	A	887	LEU	4.3
1	A	1295	PHE	4.3
1	B	985	LEU	4.3
1	A	2086	ALA	4.2
1	B	982	VAL	4.2
1	A	1694	PRO	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	945	LEU	4.1
1	A	1735	GLY	4.1
1	B	1685	ASN	4.1
1	A	2116	MET	4.1
1	B	2076	TYR	4.0
1	B	1369	PHE	4.0
1	A	985	LEU	4.0
1	B	1604	MET	4.0
1	A	889	ASP	4.0
1	A	2233	TYR	4.0
1	A	2002	ARG	4.0
1	B	1204	LEU	3.9
1	B	1256	ASN	3.9
1	B	934	ALA	3.8
1	B	2179	ARG	3.8
1	A	1755	THR	3.7
1	A	1293	LEU	3.7
1	A	1553	PHE	3.7
1	B	2089	ASP	3.7
1	B	887	LEU	3.6
1	B	2130	ILE	3.6
1	B	2240	ILE	3.6
1	A	929	LEU	3.5
1	A	1703	LEU	3.5
1	A	2222	PHE	3.5
1	A	1711	PHE	3.5
1	A	2134	PHE	3.5
1	A	1254	VAL	3.5
1	A	2255	GLN	3.5
1	B	1255	VAL	3.5
1	A	2005	TYR	3.5
1	B	2007	GLU	3.5
1	B	978	LYS	3.4
1	A	2109	SER	3.4
1	A	2127	TYR	3.4
1	A	1574	LYS	3.4
1	B	949	GLU	3.4
1	A	2176	ILE	3.4
1	A	1971	PHE	3.3
1	A	1649	PHE	3.3
1	B	1945	PRO	3.3
1	B	2163	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	947	ASP	3.3
1	B	969	VAL	3.2
1	A	1733	ILE	3.2
1	B	2084	THR	3.2
1	A	845	PHE	3.2
1	B	971	SER	3.2
1	A	1507	VAL	3.2
1	B	1733	ILE	3.2
1	A	2257	ARG	3.2
1	B	1509	GLY	3.1
1	A	971	SER	3.1
1	B	2039	GLY	3.1
1	A	904	LEU	3.1
1	A	838	TYR	3.1
1	B	2038	GLY	3.1
1	B	2002	ARG	3.1
1	A	839	SER	3.0
1	A	969	VAL	3.0
1	A	1159	THR	3.0
1	A	1944	THR	3.0
1	A	1714	GLU	2.9
1	B	2088	LEU	2.9
1	A	1991	LEU	2.9
1	B	938	CYS	2.9
1	A	1619	PRO	2.9
1	A	1326	PRO	2.9
1	A	907	LEU	2.9
1	B	2260	LEU	2.9
1	B	804	TYR	2.8
1	A	1901	LEU	2.8
1	B	2011	TYR	2.8
1	A	1208	LEU	2.8
1	A	1843	ILE	2.8
1	A	1734	VAL	2.8
1	B	1979	ASP	2.8
1	A	2113	LYS	2.8
1	B	975	VAL	2.7
1	A	1677	ALA	2.7
1	B	1494	GLU	2.7
1	A	1887	MET	2.7
1	B	2113	LYS	2.7
1	B	1911	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1616	ALA	2.7
1	A	2252	ILE	2.7
1	A	1105	TYR	2.6
1	B	1208	LEU	2.6
1	A	895	THR	2.6
1	B	827	PHE	2.6
1	A	1331	GLN	2.6
1	B	1013	LEU	2.6
1	B	2127	TYR	2.6
1	B	1603	GLY	2.6
1	A	2106	LYS	2.5
1	A	2110	ASP	2.5
1	B	1174	MET	2.5
1	B	2133	GLN	2.5
1	A	1364	THR	2.5
1	B	805	GLY	2.5
1	A	968	THR	2.5
1	B	1619	PRO	2.5
1	B	828	ILE	2.5
1	B	1602	PRO	2.5
1	A	1327	SER	2.4
1	A	840	GLU	2.4
1	B	941	SER	2.4
1	B	1526	PRO	2.4
1	B	840	GLU	2.4
1	A	2091	VAL	2.4
1	A	2253	ALA	2.4
1	A	824	LEU	2.4
1	B	1436	LEU	2.4
1	B	808	CYS	2.3
1	B	2244	LEU	2.3
1	B	940	PHE	2.3
1	A	1888	ILE	2.3
1	A	2123	LEU	2.3
1	B	1105	TYR	2.3
1	B	1984	GLU	2.3
1	A	1104	VAL	2.3
1	B	2116	MET	2.3
1	A	2011	TYR	2.3
1	B	1830	HIS	2.3
1	B	1285	LEU	2.3
1	B	1861	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1597	GLU	2.2
1	A	1363	GLU	2.2
1	A	1676	LEU	2.2
1	B	1182	ARG	2.2
1	A	2240	ILE	2.2
1	B	2010	LYS	2.2
1	A	1475	LEU	2.2
1	B	2180	ILE	2.2
1	A	1257	VAL	2.2
1	A	1454	GLN	2.2
1	A	1587	LEU	2.1
1	A	837	PRO	2.1
1	B	1564	ALA	2.1
1	A	1918	VAL	2.1
1	A	1174	MET	2.1
1	B	1529	ASN	2.1
1	B	1683	HIS	2.1
1	B	1295	PHE	2.1
1	A	1917	THR	2.1
1	B	1730	ILE	2.1
1	B	2253	ALA	2.1
1	B	913	LEU	2.1
1	A	1325	GLU	2.1
1	A	1557	ILE	2.0
1	A	1428	THR	2.0
1	B	1018	SER	2.0
1	B	974	ASN	2.0
1	A	888	ASP	2.0
1	B	800	PHE	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 ⓘ

There are no such residues in this entry.