



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:45 am BST

PDB ID : 5G1P
Title : Aspartate transcarbamoylase domain of human CAD bound to carbamoyl phosphate
Authors : Ruiz-Ramos, A.; Grande-Garcia, A.; Moreno-Morcillo, M.D.; Ramon-Maiques, S.
Deposited on : 2016-03-29
Resolution : 3.19 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

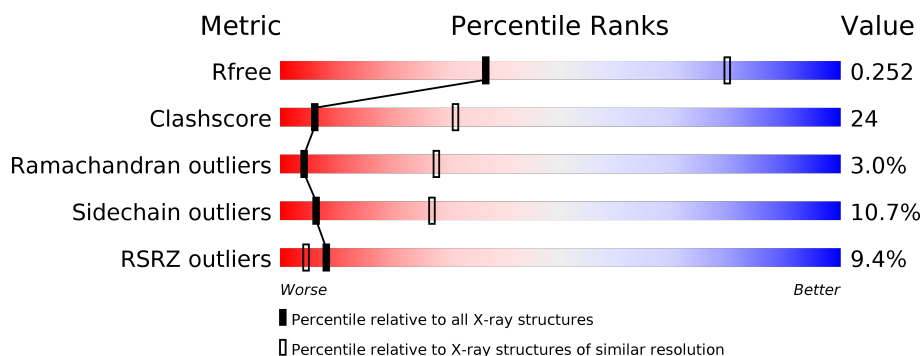
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	314	<div> <div>9%</div> <div>49% 38% 6% 7%</div> </div>
1	B	314	<div> <div>8%</div> <div>50% 36% 5% 8%</div> </div>
1	C	314	<div> <div>10%</div> <div>49% 38% 5% 8%</div> </div>
1	D	314	<div> <div>11%</div> <div>51% 38% • 7%</div> </div>
1	E	314	<div> <div>6%</div> <div>54% 35% 6% • 5%</div> </div>
1	F	314	<div> <div>10%</div> <div>53% 37% 6% • •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CP	D	3226	-	-	X	-
2	CP	F	3226	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13193 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 CAD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2175	1363	385	407	20			
1	B	288	Total	C	N	O	S	0	0	0
			2128	1337	378	393	20			
1	C	288	Total	C	N	O	S	0	0	0
			2141	1344	384	394	19			
1	D	292	Total	C	N	O	S	0	0	0
			2171	1365	384	401	21			
1	E	299	Total	C	N	O	S	0	0	0
			2197	1380	396	401	20			
1	F	304	Total	C	N	O	S	0	0	0
			2238	1407	400	414	17			

There are 18 discrepancies between the modelled and reference sequences:

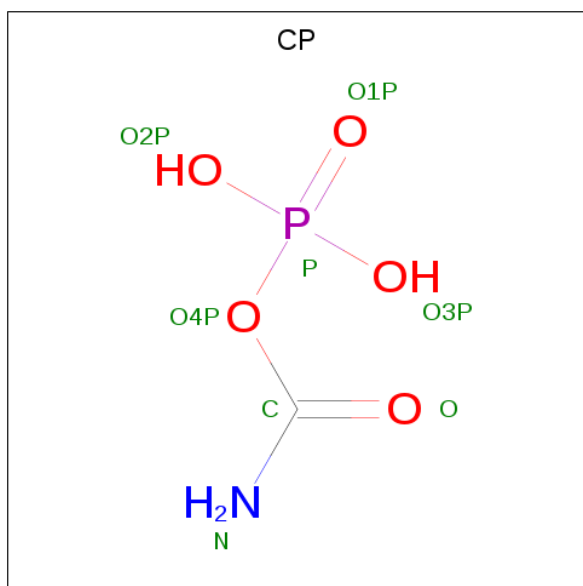
Chain	Residue	Modelled	Actual	Comment	Reference
A	1912	GLY	-	expression tag	UNP P27708
A	1913	PRO	-	expression tag	UNP P27708
A	1914	MET	-	expression tag	UNP P27708
B	1912	GLY	-	expression tag	UNP P27708
B	1913	PRO	-	expression tag	UNP P27708
B	1914	MET	-	expression tag	UNP P27708
C	1912	GLY	-	expression tag	UNP P27708
C	1913	PRO	-	expression tag	UNP P27708
C	1914	MET	-	expression tag	UNP P27708
D	1912	GLY	-	expression tag	UNP P27708
D	1913	PRO	-	expression tag	UNP P27708
D	1914	MET	-	expression tag	UNP P27708
E	1912	GLY	-	expression tag	UNP P27708
E	1913	PRO	-	expression tag	UNP P27708
E	1914	MET	-	expression tag	UNP P27708
F	1912	GLY	-	expression tag	UNP P27708
F	1913	PRO	-	expression tag	UNP P27708

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	1914	MET	-	expression tag	UNP P27708

- Molecule 2 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula: $\text{CH}_4\text{NO}_5\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			8	1	1	5	1		

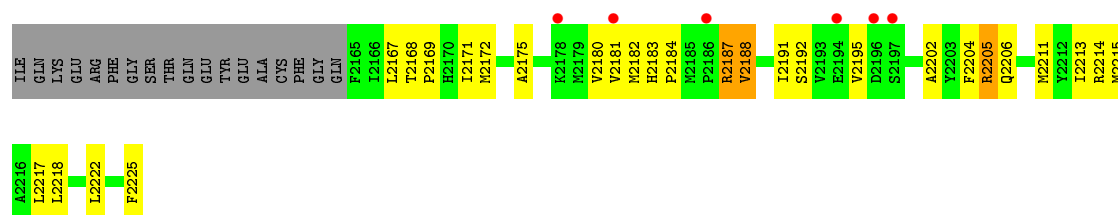
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	14	Total	O	0	0
			14	14		

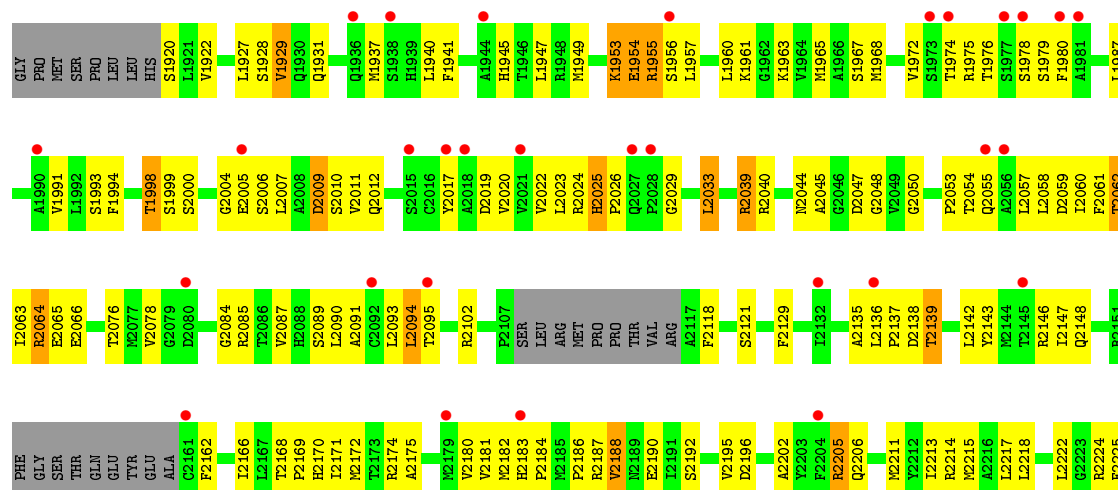
Continued on next page...

Continued from previous page...

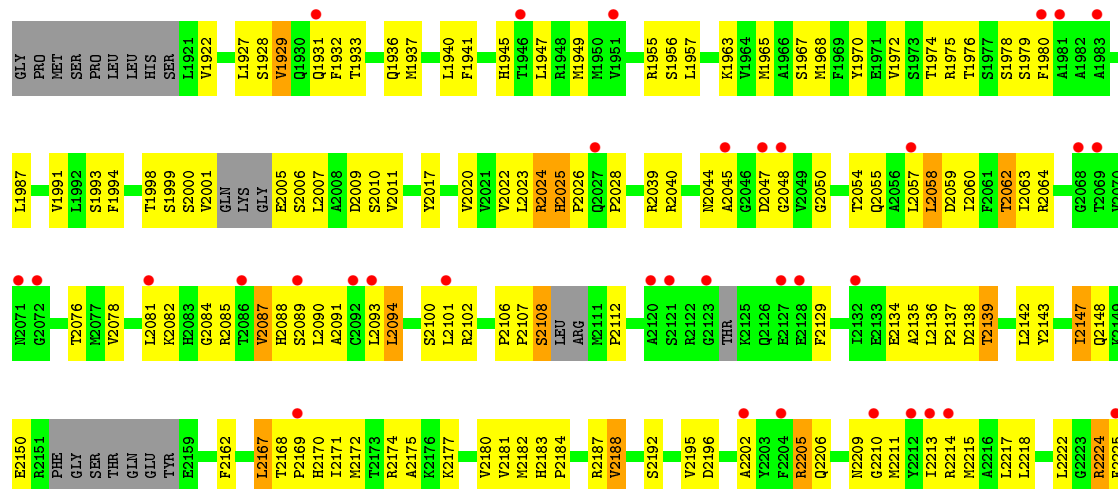
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	13	Total 13	O 13	0	0
3	D	15	Total 15	O 15	0	0
3	E	22	Total 22	O 22	0	0
3	F	15	Total 15	O 15	0	0



• Molecule 1: CAD PROTEIN

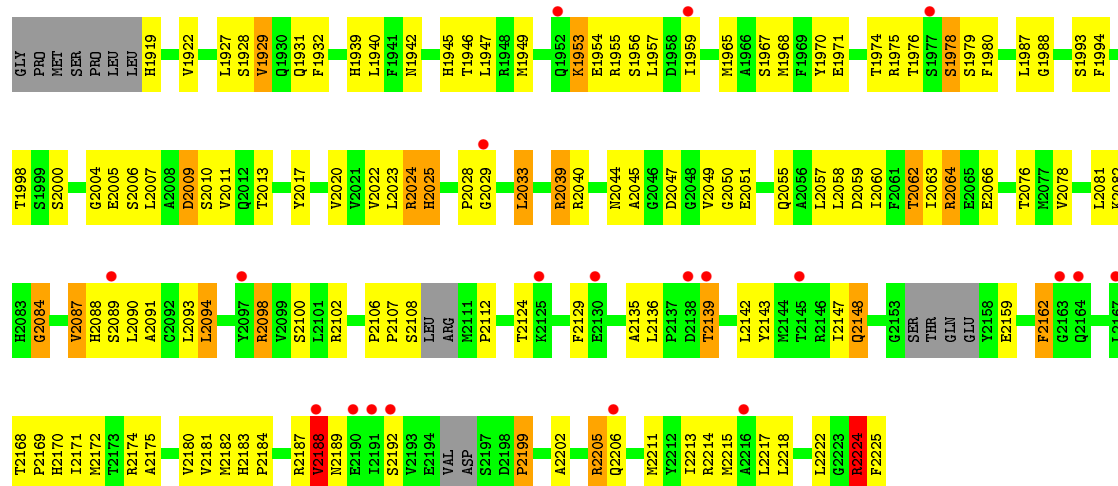


• Molecule 1: CAD PROTEIN

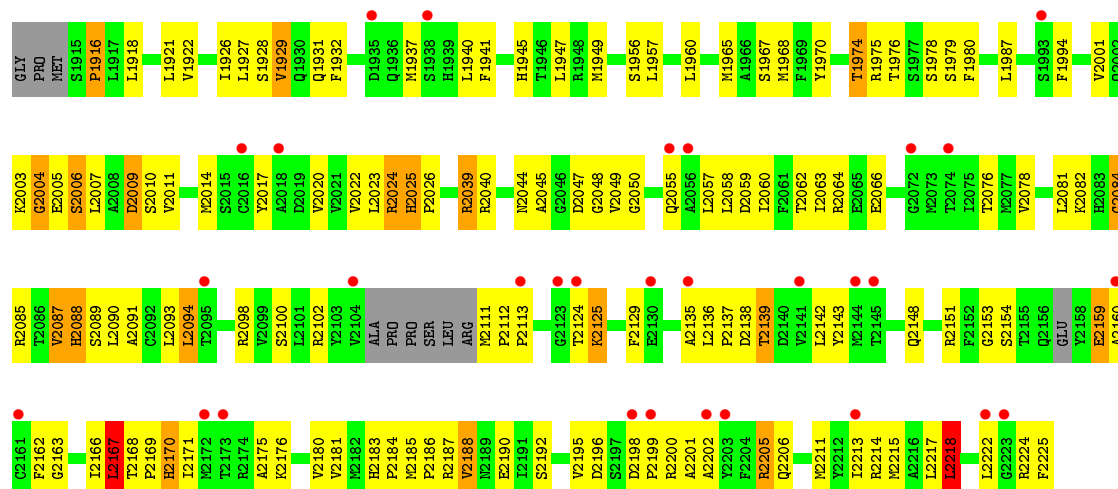


• Molecule 1: CAD PROTEIN





• Molecule 1: CAD PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.67Å 157.67Å 83.54Å 90.00° 120.08° 90.00°	Depositor
Resolution (Å)	42.54 – 3.19 42.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.54-3.19) 99.3 (42.53-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.221 , 0.251 0.222 , 0.252	Depositor DCC
R_{free} test set	1545 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.349 for l,k,-h-l 0.349 for -h-l,k,h 0.388 for l,-k,h 0.338 for -h-l,-k,l 0.408 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.284 for H, K, L 0.225 for H, -K, -H-L 0.188 for L, -K, H 0.119 for L, K, -H-L 0.099 for -H-L, K, H 0.085 for H+L, -K, -L	Depositor
Outliers	0 of 30893 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	13193	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CP

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	0.60	0/2209	0.89	7/2992 (0.2%)
1	B	0.61	0/2164	0.90	10/2937 (0.3%)
1	C	0.60	0/2174	0.89	6/2943 (0.2%)
1	D	0.60	0/2206	0.94	12/2986 (0.4%)
1	E	0.61	0/2234	1.05	10/3028 (0.3%)
1	F	0.60	0/2274	0.92	11/3083 (0.4%)
All	All	0.60	0/13261	0.93	56/17969 (0.3%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2024	ARG	NE-CZ-NH1	22.40	131.50	120.30
1	E	2024	ARG	NE-CZ-NH2	-21.46	109.57	120.30
1	F	2064	ARG	NE-CZ-NH1	12.47	126.54	120.30
1	D	2064	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	A	2205	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	B	2205	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	F	2205	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	D	2058	LEU	CB-CG-CD1	9.97	127.95	111.00
1	C	2205	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	F	2064	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	D	2064	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	D	2058	LEU	CA-CB-CG	8.61	135.11	115.30
1	B	2187	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	2205	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	E	2205	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	2064	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	D	2138	ASP	CB-CG-OD2	7.70	125.23	118.30
1	C	2205	ARG	NE-CZ-NH2	-7.55	116.52	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2064	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	2064	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	C	2064	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	E	2064	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	D	2058	LEU	CB-CG-CD2	-7.29	98.61	111.00
1	C	2064	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	2024	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	E	2039	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	2098	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	F	2218	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	B	2024	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	D	2205	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	2205	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	D	2024	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	2024	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	2138	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	E	2098	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	2024	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	D	2094	LEU	CB-CG-CD1	6.16	121.47	111.00
1	F	1916	PRO	N-CA-CB	6.12	110.65	103.30
1	F	2024	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	2064	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	F	2098	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	F	2218	LEU	CA-CB-CG	6.07	129.26	115.30
1	B	2064	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	2024	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	2039	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	2205	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	2224	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	2098	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	2024	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	2040	ARG	CG-CD-NE	5.41	123.17	111.80
1	F	2167	LEU	CA-CB-CG	5.38	127.68	115.30
1	F	2024	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	2187	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	2224	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	2058	LEU	CB-CA-C	-5.10	100.52	110.20
1	A	2036	LYS	CA-CB-CG	5.07	124.54	113.40

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	2175	0	2130	117	1
1	B	2128	0	2084	102	0
1	C	2141	0	2109	120	0
1	D	2171	0	2116	113	1
1	E	2197	0	2110	101	0
1	F	2238	0	2149	115	0
2	A	8	0	2	0	0
2	B	8	0	2	0	0
2	C	8	0	2	2	0
2	D	8	0	2	4	0
2	E	8	0	2	1	0
2	F	8	0	2	4	0
3	A	16	0	0	1	0
3	B	14	0	0	0	0
3	C	13	0	0	0	0
3	D	15	0	0	1	0
3	E	22	0	0	1	0
3	F	15	0	0	0	0
All	All	13193	0	12710	632	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (632) 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:A:2032:GLU:OE1	3:A:4009:HOH:O	1.59	1.16
1:F:2066:GLU:OE2	1:F:2205:ARG:NH1	1.82	1.13
1:E:2084:GLY:O	1:E:2088:HIS:NE2	1.85	1.10
1:A:2063:ILE:O	1:A:2067:LEU:HD12	1.52	1.08
1:E:2076:THR:OG1	1:E:2139:THR:OG1	1.74	1.04
1:D:2058:LEU:HD21	1:D:2210:GLY:CA	1.87	1.04
1:D:2076:THR:OG1	1:D:2139:THR:OG1	1.74	1.04
1:D:2167:LEU:HD11	1:D:2172:MET:HG2	1.40	1.04
1:B:2076:THR:OG1	1:B:2139:THR:OG1	1.76	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2076:THR:OG1	1:A:2139:THR:OG1	1.75	1.02
1:C:2055:GLN:OE1	2:C:3226:CP:N	1.94	1.00
1:F:2084:GLY:O	1:F:2088:HIS:NE2	1.93	1.00
1:F:2076:THR:OG1	1:F:2139:THR:OG1	1.77	1.00
1:C:2076:THR:OG1	1:C:2139:THR:OG1	1.77	1.00
1:D:2058:LEU:HD21	1:D:2210:GLY:HA3	1.45	0.99
1:A:1995:SER:OG	1:A:1998:THR:CG2	2.14	0.95
1:B:2066:GLU:OE2	1:B:2205:ARG:NH2	2.02	0.93
1:C:2061:PHE:CE2	1:C:2065:GLU:OE2	2.22	0.92
1:F:2111:MET:O	1:F:2113:PRO:HD3	1.72	0.90
1:C:2066:GLU:OE2	1:C:2205:ARG:NH2	2.05	0.89
1:D:2102:ARG:NH1	1:D:2135:ALA:O	2.06	0.89
1:F:2102:ARG:NH1	1:F:2135:ALA:O	2.06	0.88
1:C:2102:ARG:NH1	1:C:2135:ALA:O	2.06	0.87
1:E:2169:PRO:HD3	1:E:2192:SER:CB	2.05	0.87
1:E:2102:ARG:NH1	1:E:2135:ALA:O	2.06	0.86
1:D:2058:LEU:CD2	1:D:2210:GLY:CA	2.53	0.86
1:A:1995:SER:OG	1:A:1998:THR:HG23	1.75	0.85
1:A:2066:GLU:OE2	1:A:2205:ARG:NH2	2.11	0.82
1:C:2146:ARG:HH21	1:C:2186:PRO:HG2	1.41	0.82
1:F:2142:LEU:HD23	1:F:2167:LEU:HD11	1.62	0.79
1:D:2058:LEU:CD2	1:D:2210:GLY:HA2	2.12	0.79
1:F:1975:ARG:HB3	2:F:3226:CP:O4P	1.83	0.78
1:A:2146:ARG:NH2	1:B:2003:LYS:O	2.16	0.78
1:D:1975:ARG:NH2	1:E:2005:GLU:OE2	2.17	0.78
1:E:2159:GLU:HA	1:E:2162:PHE:HB2	1.66	0.78
1:E:2084:GLY:O	1:E:2088:HIS:CD2	2.37	0.77
1:F:1921:LEU:HD22	1:F:1926:ILE:HD11	1.67	0.76
1:A:2074:THR:HG21	1:A:2138:ASP:O	1.84	0.76
1:A:1974:THR:HG21	1:B:1999:SER:HB2	1.67	0.76
1:F:1979:SER:OG	1:F:2214:ARG:NH1	2.19	0.76
1:A:1979:SER:OG	1:A:2214:ARG:NH1	2.20	0.75
1:C:1979:SER:OG	1:C:2214:ARG:NH1	2.19	0.75
1:E:1979:SER:OG	1:E:2214:ARG:NH1	2.20	0.75
1:A:2063:ILE:O	1:A:2067:LEU:CD1	2.32	0.75
1:A:1995:SER:OG	1:A:1998:THR:HG22	1.86	0.74
1:D:1979:SER:OG	1:D:2214:ARG:NH1	2.20	0.74
1:B:1979:SER:OG	1:B:2214:ARG:NH1	2.20	0.73
1:A:2050:GLY:O	1:A:2085:ARG:O	2.05	0.73
1:E:1975:ARG:NH1	2:E:3226:CP:O1P	2.21	0.73
1:D:2088:HIS:NE2	1:D:2112:PRO:HG2	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2120:ALA:HB2	1:A:2126:GLN:OE1	1.92	0.70
1:F:2050:GLY:HA2	1:F:2085:ARG:HD2	1.74	0.70
1:C:2087:VAL:CG1	1:C:2143:TYR:CE1	2.75	0.69
1:C:2039:ARG:O	1:C:2040:ARG:NH1	2.25	0.69
1:D:2039:ARG:O	1:D:2040:ARG:NH1	2.25	0.69
1:A:2098:ARG:HH11	1:A:2098:ARG:HG3	1.56	0.68
1:F:2039:ARG:O	1:F:2040:ARG:NH1	2.26	0.68
1:A:2017:TYR:CE1	1:C:1979:SER:HB3	2.29	0.68
1:D:2094:LEU:HD13	1:D:2101:LEU:HD21	1.76	0.68
1:A:2039:ARG:O	1:A:2040:ARG:NH1	2.27	0.68
1:C:1920:SER:OG	1:C:1920:SER:O	2.09	0.68
1:E:2066:GLU:OE2	1:E:2205:ARG:NH1	2.28	0.67
1:D:1979:SER:HB3	1:E:2017:TYR:CE1	2.29	0.67
1:C:2061:PHE:CZ	1:C:2065:GLU:OE2	2.49	0.66
1:A:2192:SER:O	1:A:2195:VAL:HG23	1.95	0.66
1:D:1933:THR:OG1	1:D:1936:GLN:NE2	2.28	0.66
1:E:2039:ARG:O	1:E:2040:ARG:NH1	2.29	0.66
1:A:1940:LEU:CD2	1:A:2057:LEU:HD22	2.26	0.65
1:B:2192:SER:O	1:B:2195:VAL:HG23	1.97	0.65
1:C:2192:SER:O	1:C:2195:VAL:HG23	1.97	0.65
1:D:2192:SER:O	1:D:2195:VAL:HG23	1.97	0.65
1:F:2050:GLY:O	1:F:2085:ARG:O	2.13	0.65
1:B:2084:GLY:O	1:B:2088:HIS:CE1	2.51	0.64
1:F:2192:SER:O	1:F:2195:VAL:HG23	1.96	0.64
1:A:2020:VAL:HG13	1:A:2222:LEU:HD21	1.80	0.64
1:A:1940:LEU:HD23	1:A:2057:LEU:HD22	1.78	0.64
1:F:2020:VAL:HG13	1:F:2222:LEU:HD21	1.80	0.64
1:B:2126:GLN:O	1:B:2126:GLN:HG2	1.98	0.64
1:D:2007:LEU:O	1:D:2011:VAL:HG23	1.98	0.64
1:B:2007:LEU:O	1:B:2011:VAL:HG23	1.99	0.63
1:B:2120:ALA:HA	1:B:2126:GLN:HE22	1.63	0.63
1:C:1953:LYS:O	1:C:1954:GLU:HB3	1.98	0.63
1:E:2020:VAL:HG13	1:E:2222:LEU:HD21	1.80	0.63
1:E:2224:ARG:N	1:E:2224:ARG:HD2	2.13	0.63
1:A:2007:LEU:O	1:A:2011:VAL:HG23	1.98	0.63
1:C:1955:ARG:HD2	1:E:2199:PRO:HB3	1.80	0.63
1:B:1974:THR:HG21	1:C:1999:SER:HB2	1.79	0.63
1:C:1940:LEU:HD21	1:C:2057:LEU:HD21	1.81	0.63
1:C:2061:PHE:CD1	1:C:2065:GLU:HG3	2.34	0.63
1:E:2007:LEU:O	1:E:2011:VAL:HG23	1.98	0.63
1:C:2007:LEU:O	1:C:2011:VAL:HG23	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2187:ARG:NH2	1:F:2196:ASP:OD1	2.32	0.62
1:E:1988:GLY:HA2	3:E:4010:HOH:O	1.99	0.62
1:A:2074:THR:CG2	1:A:2138:ASP:O	2.47	0.62
1:F:1940:LEU:CD2	1:F:2057:LEU:HD22	2.29	0.62
1:F:1940:LEU:HD23	1:F:2057:LEU:HD22	1.80	0.62
1:A:2033:LEU:O	1:A:2036:LYS:HB2	1.99	0.62
1:B:2000:SER:O	1:B:2004:GLY:N	2.32	0.62
1:C:2020:VAL:HG13	1:C:2222:LEU:HD21	1.81	0.62
1:B:1979:SER:HB3	1:C:2017:TYR:CE1	2.34	0.62
1:C:1940:LEU:HD21	1:C:2057:LEU:CD2	2.30	0.62
1:F:1975:ARG:N	2:F:3226:CP:O1P	2.33	0.62
1:D:1940:LEU:CD2	1:D:2057:LEU:HD22	2.30	0.61
1:E:1932:PHE:CZ	1:E:2057:LEU:HD11	2.35	0.61
1:F:2007:LEU:O	1:F:2011:VAL:HG23	1.99	0.61
1:B:1934:LYS:O	1:B:1938:SER:OG	2.14	0.61
1:E:1940:LEU:HD23	1:E:2057:LEU:HD22	1.82	0.61
1:A:1979:SER:HB3	1:B:2017:TYR:CE1	2.35	0.61
1:D:1999:SER:O	1:D:2001:VAL:N	2.32	0.61
1:A:1932:PHE:CZ	1:A:2057:LEU:HD11	2.36	0.61
1:D:1940:LEU:HD23	1:D:2057:LEU:HD22	1.81	0.61
1:A:2029:GLY:O	1:A:2033:LEU:HD23	2.01	0.61
1:B:1940:LEU:CD2	1:B:2057:LEU:HD22	2.31	0.61
1:B:1940:LEU:HD23	1:B:2057:LEU:HD22	1.81	0.61
1:E:1959:ILE:O	1:E:2224:ARG:HG2	2.00	0.61
1:B:2183:HIS:CE1	1:B:2187:ARG:HB3	2.36	0.61
1:C:2029:GLY:O	1:C:2033:LEU:HD23	2.01	0.60
1:E:1940:LEU:CD2	1:E:2057:LEU:HD22	2.31	0.60
1:F:1932:PHE:CZ	1:F:2057:LEU:HD11	2.36	0.60
1:D:2020:VAL:HG13	1:D:2222:LEU:HD21	1.81	0.60
1:E:1971:GLU:HB2	1:E:2024:ARG:HD3	1.82	0.60
1:E:2188:VAL:HG13	1:F:2004:GLY:O	2.00	0.60
1:F:1929:VAL:CG1	1:F:2093:LEU:HD22	2.31	0.60
1:E:2029:GLY:O	1:E:2033:LEU:HD23	2.02	0.60
1:B:2029:GLY:O	1:B:2033:LEU:HD23	2.01	0.60
1:C:2187:ARG:NH2	1:C:2196:ASP:OD1	2.33	0.60
1:D:1963:LYS:HE2	1:D:2224:ARG:HH12	1.67	0.60
1:E:1971:GLU:OE1	1:E:2024:ARG:HD3	2.02	0.60
1:F:1921:LEU:HD22	1:F:1926:ILE:CD1	2.32	0.60
1:C:2118:PHE:O	1:C:2121:SER:OG	2.20	0.59
1:A:1929:VAL:HG23	1:A:2051:GLU:OE1	2.03	0.59
1:B:2020:VAL:HG13	1:B:2222:LEU:HD21	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1929:VAL:HG12	1:F:2093:LEU:HD22	1.84	0.59
1:D:2167:LEU:HD12	1:D:2167:LEU:C	2.21	0.59
1:A:2214:ARG:N	1:A:2214:ARG:HD2	2.18	0.59
1:D:1932:PHE:CZ	1:D:2057:LEU:HD11	2.38	0.59
1:E:1979:SER:HB3	1:F:2017:TYR:CE1	2.38	0.59
1:E:2143:TYR:CZ	1:E:2184:PRO:HD3	2.38	0.59
1:C:2050:GLY:O	1:C:2085:ARG:O	2.21	0.59
1:D:2168:THR:HB	1:D:2169:PRO:HD2	1.85	0.59
1:B:1957:LEU:O	1:B:1987:LEU:O	2.22	0.58
1:D:2058:LEU:HD23	1:D:2210:GLY:HA2	1.85	0.58
1:A:1929:VAL:CG1	1:A:2093:LEU:HD22	2.34	0.58
1:B:1932:PHE:CZ	1:B:2057:LEU:HD11	2.39	0.58
1:D:2170:HIS:ND1	1:D:2170:HIS:O	2.37	0.58
1:F:1957:LEU:O	1:F:1987:LEU:O	2.22	0.58
1:D:1957:LEU:O	1:D:1987:LEU:O	2.22	0.58
1:C:1929:VAL:HG12	1:C:2093:LEU:HD22	1.86	0.58
1:D:2050:GLY:O	1:D:2085:ARG:O	2.21	0.58
1:D:1929:VAL:HG12	1:D:2093:LEU:HD22	1.86	0.58
1:E:1929:VAL:CG1	1:E:2093:LEU:HD22	2.33	0.58
1:A:2102:ARG:NH1	1:A:2129:PHE:CZ	2.72	0.58
1:B:2050:GLY:O	1:B:2085:ARG:O	2.22	0.58
1:E:1928:SER:O	1:E:1931:GLN:HG2	2.03	0.58
1:E:1929:VAL:HG12	1:E:2093:LEU:HD22	1.86	0.58
1:F:2059:ASP:O	1:F:2063:ILE:HG13	2.04	0.58
1:C:1929:VAL:CG1	1:C:2093:LEU:HD22	2.33	0.58
1:A:1957:LEU:O	1:A:1987:LEU:O	2.22	0.57
1:B:2059:ASP:O	1:B:2063:ILE:HG13	2.04	0.57
1:C:1957:LEU:O	1:C:1987:LEU:O	2.21	0.57
1:D:2167:LEU:CD1	1:D:2168:THR:O	2.52	0.57
1:A:1928:SER:O	1:A:1931:GLN:HG2	2.03	0.57
1:D:1929:VAL:CG1	1:D:2093:LEU:HD22	2.34	0.57
1:D:2187:ARG:NH2	1:D:2196:ASP:OD1	2.32	0.57
1:F:2143:TYR:CZ	1:F:2184:PRO:HD3	2.39	0.57
1:C:2143:TYR:CZ	1:C:2184:PRO:HD3	2.40	0.57
1:F:2084:GLY:O	1:F:2088:HIS:CD2	2.56	0.57
1:B:1929:VAL:HG12	1:B:2093:LEU:HD22	1.87	0.57
1:B:1928:SER:O	1:B:1931:GLN:HG2	2.05	0.57
1:E:1957:LEU:O	1:E:1987:LEU:O	2.22	0.57
1:E:1949:MET:O	1:E:1953:LYS:HD2	2.05	0.57
1:B:1929:VAL:CG1	1:B:2093:LEU:HD22	2.35	0.57
1:B:2143:TYR:CZ	1:B:2184:PRO:HD3	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1933:THR:H	1:D:1936:GLN:HE21	1.53	0.56
1:D:2059:ASP:O	1:D:2063:ILE:HG13	2.05	0.56
1:A:1929:VAL:HG12	1:A:2093:LEU:HD22	1.87	0.56
1:C:1928:SER:O	1:C:1931:GLN:HG2	2.04	0.56
1:F:2214:ARG:N	1:F:2214:ARG:HD2	2.20	0.56
1:D:1928:SER:O	1:D:1931:GLN:HG2	2.05	0.56
1:D:2024:ARG:HH12	2:D:3226:CP:P	2.28	0.56
1:E:2214:ARG:HD2	1:E:2214:ARG:N	2.19	0.56
1:D:2054:THR:O	1:D:2213:ILE:CD1	2.53	0.56
1:A:2060:ILE:HD12	1:A:2090:LEU:HD11	1.88	0.56
1:F:2142:LEU:HD23	1:F:2167:LEU:CD1	2.33	0.56
1:C:2061:PHE:CD2	1:C:2065:GLU:OE2	2.58	0.56
1:D:2005:GLU:OE1	1:F:2186:PRO:HB3	2.06	0.56
1:D:2078:VAL:HG21	1:D:2142:LEU:HD11	1.88	0.56
1:F:1928:SER:O	1:F:1931:GLN:HG2	2.05	0.56
1:A:1974:THR:CG2	1:B:1999:SER:HB2	2.35	0.55
1:B:2054:THR:O	1:B:2213:ILE:CD1	2.54	0.55
1:C:2059:ASP:OD1	1:C:2206:GLN:NE2	2.39	0.55
1:A:2129:PHE:CD2	1:A:2135:ALA:HB2	2.41	0.55
1:B:2078:VAL:HG21	1:B:2142:LEU:HD11	1.88	0.55
1:D:2059:ASP:OD1	1:D:2206:GLN:NE2	2.39	0.55
1:D:2214:ARG:HD2	1:D:2214:ARG:N	2.22	0.55
1:F:2198:ASP:O	1:F:2199:PRO:C	2.44	0.55
1:A:2169:PRO:HD3	1:A:2192:SER:HB3	1.88	0.55
1:E:2059:ASP:O	1:E:2063:ILE:HG13	2.06	0.55
1:F:2060:ILE:HD12	1:F:2090:LEU:HD11	1.89	0.55
1:F:2078:VAL:HG21	1:F:2142:LEU:HD11	1.89	0.55
1:C:2169:PRO:HD3	1:C:2192:SER:HB3	1.88	0.55
1:C:2054:THR:O	1:C:2213:ILE:CD1	2.55	0.55
1:C:2087:VAL:HG12	1:C:2143:TYR:CE1	2.41	0.55
1:A:2059:ASP:O	1:A:2063:ILE:HG13	2.07	0.55
1:B:2183:HIS:HD2	1:B:2184:PRO:HD2	1.72	0.55
1:C:2061:PHE:CE1	1:C:2065:GLU:HG3	2.42	0.55
1:F:2024:ARG:NH1	2:F:3226:CP:O3P	2.36	0.55
1:B:2214:ARG:HD2	1:B:2214:ARG:N	2.22	0.55
1:D:2060:ILE:HD12	1:D:2090:LEU:HD11	1.88	0.55
1:E:2059:ASP:OD1	1:E:2206:GLN:NE2	2.40	0.55
1:F:2050:GLY:HA2	1:F:2085:ARG:CD	2.37	0.55
1:B:2059:ASP:OD1	1:B:2206:GLN:NE2	2.40	0.54
1:D:2143:TYR:CZ	1:D:2184:PRO:HD3	2.42	0.54
1:E:2084:GLY:O	1:E:2088:HIS:CE1	2.59	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1965:MET:HG3	1:E:2020:VAL:HG23	1.89	0.54
1:A:2078:VAL:HG21	1:A:2142:LEU:HD11	1.90	0.54
1:A:2098:ARG:HH11	1:A:2098:ARG:CG	2.19	0.54
1:A:2143:TYR:CZ	1:A:2184:PRO:HD3	2.42	0.54
1:E:2000:SER:O	1:E:2004:GLY:N	2.40	0.54
1:B:2187:ARG:NH1	1:B:2191:ILE:O	2.40	0.54
1:C:2214:ARG:HD2	1:C:2214:ARG:N	2.22	0.54
1:E:2180:VAL:CG2	1:E:2202:ALA:HB3	2.38	0.54
1:F:2059:ASP:OD1	1:F:2206:GLN:NE2	2.41	0.54
1:C:1953:LYS:O	1:C:1954:GLU:CB	2.56	0.54
1:A:2062:THR:HB	1:A:2182:MET:HE3	1.90	0.54
1:C:1965:MET:HG3	1:C:2020:VAL:HG23	1.89	0.54
1:F:2136:LEU:HD12	1:F:2139:THR:HG21	1.90	0.54
1:C:2005:GLU:OE2	1:C:2009:ASP:HB3	2.07	0.54
1:D:2054:THR:O	1:D:2213:ILE:HD11	2.08	0.54
1:C:2162:PHE:O	1:C:2166:ILE:HG13	2.07	0.53
1:F:2058:LEU:HB3	1:F:2213:ILE:HG13	1.90	0.53
1:C:2060:ILE:HD12	1:C:2090:LEU:HD11	1.89	0.53
1:B:2054:THR:O	1:B:2213:ILE:HD11	2.07	0.53
1:C:2059:ASP:O	1:C:2063:ILE:HG13	2.07	0.53
1:F:2084:GLY:O	1:F:2088:HIS:CE1	2.59	0.53
1:A:1965:MET:HG3	1:A:2020:VAL:HG23	1.89	0.53
1:D:2055:GLN:O	1:D:2058:LEU:HB2	2.09	0.53
1:E:2060:ILE:HD12	1:E:2090:LEU:HD11	1.90	0.53
1:F:2170:HIS:ND1	1:F:2170:HIS:O	2.42	0.53
1:B:2060:ILE:HD12	1:B:2090:LEU:HD11	1.89	0.53
1:A:2000:SER:OG	1:C:1974:THR:HG22	2.08	0.53
1:E:2136:LEU:HD21	1:E:2175:ALA:HB2	1.90	0.53
1:E:2078:VAL:HG21	1:E:2142:LEU:HD11	1.90	0.53
1:F:2136:LEU:HD21	1:F:2175:ALA:HB2	1.90	0.53
1:F:2213:ILE:O	1:F:2217:LEU:N	2.41	0.53
1:A:2170:HIS:O	1:A:2170:HIS:ND1	2.41	0.53
1:B:2098:ARG:CG	1:B:2098:ARG:HH11	2.21	0.53
1:C:2078:VAL:HG21	1:C:2142:LEU:HD11	1.91	0.53
1:E:2170:HIS:O	1:E:2170:HIS:ND1	2.42	0.53
1:A:2059:ASP:OD1	1:A:2206:GLN:NE2	2.42	0.53
1:F:1968:MET:O	1:F:2023:LEU:HA	2.09	0.53
1:F:1965:MET:HG3	1:F:2020:VAL:HG23	1.90	0.53
1:A:1967:SER:O	1:A:1994:PHE:HB3	2.08	0.53
1:C:2054:THR:O	1:C:2213:ILE:HD11	2.09	0.53
1:D:1967:SER:O	1:D:1994:PHE:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1965:MET:HG3	1:B:2020:VAL:HG23	1.90	0.52
1:B:2213:ILE:HG13	1:B:2214:ARG:HD2	1.92	0.52
1:E:1967:SER:O	1:E:1994:PHE:HB3	2.08	0.52
1:A:2005:GLU:OE1	1:A:2009:ASP:HB3	2.09	0.52
1:C:2062:THR:HB	1:C:2182:MET:HE3	1.91	0.52
1:C:2136:LEU:HD12	1:C:2139:THR:HG21	1.91	0.52
1:E:2180:VAL:CG2	1:E:2202:ALA:CB	2.88	0.52
1:C:2061:PHE:CE1	1:C:2065:GLU:CG	2.92	0.52
1:F:2169:PRO:HD3	1:F:2192:SER:HB3	1.91	0.52
1:C:2000:SER:O	1:C:2004:GLY:N	2.43	0.52
1:D:2213:ILE:O	1:D:2217:LEU:N	2.42	0.52
1:C:2065:GLU:OE1	1:E:1945:HIS:CE1	2.63	0.52
1:C:2050:GLY:CA	1:C:2085:ARG:HD3	2.40	0.52
1:D:1965:MET:HG3	1:D:2020:VAL:HG23	1.90	0.52
1:E:2062:THR:HB	1:E:2182:MET:HE3	1.92	0.52
1:E:2147:ILE:O	1:E:2148:GLN:CB	2.57	0.52
1:A:1968:MET:O	1:A:2023:LEU:HA	2.10	0.52
1:A:2180:VAL:CG2	1:A:2202:ALA:CB	2.88	0.52
1:B:2167:LEU:O	1:B:2195:VAL:HG21	2.09	0.52
1:C:2050:GLY:HA2	1:C:2085:ARG:CD	2.40	0.52
1:F:2136:LEU:O	1:F:2139:THR:HB	2.10	0.52
1:F:2214:ARG:O	1:F:2218:LEU:HB2	2.10	0.51
1:A:2180:VAL:CG2	1:A:2202:ALA:HB3	2.40	0.51
1:E:2213:ILE:O	1:E:2217:LEU:N	2.41	0.51
1:B:2136:LEU:HD21	1:B:2175:ALA:HB2	1.93	0.51
1:A:2136:LEU:HD21	1:A:2175:ALA:HB2	1.92	0.51
1:B:2180:VAL:CG2	1:B:2202:ALA:HB3	2.40	0.51
1:B:1975:ARG:NH2	1:C:2005:GLU:OE1	2.43	0.51
1:A:2058:LEU:HB3	1:A:2213:ILE:HG13	1.93	0.51
1:D:2106:PRO:O	1:D:2108:SER:N	2.43	0.51
1:D:1972:VAL:HG13	1:E:1998:THR:C	2.31	0.51
1:D:2205:ARG:O	1:D:2209:ASN:ND2	2.43	0.51
1:B:1967:SER:O	1:B:1994:PHE:HB3	2.11	0.51
1:C:1968:MET:O	1:C:2023:LEU:HA	2.11	0.51
1:C:2136:LEU:O	1:C:2139:THR:HB	2.10	0.51
1:D:2017:TYR:CE1	1:F:1979:SER:HB3	2.46	0.51
1:A:2213:ILE:O	1:A:2217:LEU:N	2.43	0.51
1:B:1968:MET:O	1:B:2023:LEU:HA	2.10	0.51
1:C:2180:VAL:CG2	1:C:2202:ALA:HB3	2.41	0.51
1:D:2136:LEU:HD21	1:D:2175:ALA:HB2	1.93	0.51
1:F:2111:MET:O	1:F:2113:PRO:CD	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2014:MET:CE	1:C:1974:THR:OG1	2.59	0.50
1:B:2180:VAL:CG2	1:B:2202:ALA:CB	2.89	0.50
1:C:2146:ARG:HH21	1:C:2186:PRO:CG	2.19	0.50
1:D:1999:SER:C	1:D:2001:VAL:H	2.14	0.50
1:D:2180:VAL:CG2	1:D:2202:ALA:CB	2.89	0.50
1:D:2180:VAL:CG2	1:D:2202:ALA:HB3	2.40	0.50
1:E:1968:MET:O	1:E:2023:LEU:HA	2.11	0.50
1:A:2187:ARG:NH2	1:A:2196:ASP:OD1	2.36	0.50
1:D:2062:THR:HB	1:D:2182:MET:HE3	1.92	0.50
1:E:2047:ASP:OD1	1:E:2051:GLU:N	2.44	0.50
1:B:2213:ILE:O	1:B:2217:LEU:N	2.43	0.50
1:D:2213:ILE:HG13	1:D:2214:ARG:HD2	1.94	0.50
1:D:2024:ARG:NH1	2:D:3226:CP:O3P	2.36	0.50
1:D:1976:THR:OG1	2:D:3226:CP:O	2.29	0.50
1:B:2062:THR:HB	1:B:2182:MET:HE3	1.92	0.50
1:A:2000:SER:O	1:A:2004:GLY:N	2.45	0.50
1:B:2136:LEU:O	1:B:2139:THR:HB	2.11	0.50
1:C:2213:ILE:O	1:C:2217:LEU:N	2.42	0.50
1:D:2055:GLN:HA	1:D:2058:LEU:HD12	1.93	0.50
1:D:2183:HIS:HD2	1:D:2184:PRO:HD2	1.77	0.50
1:E:2058:LEU:HB3	1:E:2213:ILE:HG13	1.92	0.50
1:A:1934:LYS:O	1:A:1938:SER:OG	2.24	0.50
1:A:1940:LEU:CD2	1:A:2057:LEU:CD2	2.90	0.50
1:A:2081:LEU:HD22	1:A:2087:VAL:HG11	1.94	0.50
1:C:2136:LEU:HD21	1:C:2175:ALA:HB2	1.93	0.50
1:D:2088:HIS:NE2	1:D:2112:PRO:HD2	2.27	0.50
1:F:1967:SER:O	1:F:1994:PHE:HB3	2.10	0.50
1:C:2213:ILE:HG13	1:C:2214:ARG:HD2	1.93	0.49
1:D:1968:MET:O	1:D:2023:LEU:HA	2.11	0.49
1:D:2088:HIS:CE1	1:D:2112:PRO:HG2	2.47	0.49
1:B:2081:LEU:HD22	1:B:2087:VAL:HG11	1.94	0.49
1:C:2026:PRO:O	1:C:2048:GLY:CA	2.60	0.49
1:E:2058:LEU:HD12	1:E:2059:ASP:N	2.27	0.49
1:B:1972:VAL:HG13	1:C:1998:THR:C	2.32	0.49
1:C:2180:VAL:CG2	1:C:2202:ALA:CB	2.90	0.49
1:A:2014:MET:HE3	1:C:1974:THR:OG1	2.12	0.49
1:A:2136:LEU:O	1:A:2139:THR:HB	2.13	0.49
1:F:2180:VAL:CG2	1:F:2202:ALA:CB	2.91	0.49
1:F:2183:HIS:HD2	1:F:2184:PRO:HD2	1.78	0.49
1:A:2183:HIS:HD2	1:A:2184:PRO:HD2	1.78	0.49
1:B:2098:ARG:HG3	1:B:2098:ARG:HH11	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1967:SER:O	1:C:1994:PHE:HB3	2.13	0.49
1:D:2167:LEU:HD12	1:D:2168:THR:O	2.12	0.48
1:E:1971:GLU:CB	1:E:2024:ARG:HD3	2.43	0.48
1:F:2081:LEU:HD22	1:F:2087:VAL:HG11	1.95	0.48
1:A:2183:HIS:CE1	1:A:2187:ARG:HB3	2.48	0.48
1:B:1974:THR:CG2	1:C:1999:SER:HB2	2.43	0.48
1:D:2167:LEU:C	1:D:2167:LEU:CD1	2.80	0.48
1:D:2183:HIS:CE1	1:D:2187:ARG:HB3	2.49	0.48
1:F:2050:GLY:CA	1:F:2085:ARG:HD2	2.41	0.48
1:F:2180:VAL:CG2	1:F:2202:ALA:HB3	2.43	0.48
1:A:2026:PRO:O	1:A:2048:GLY:CA	2.61	0.48
1:A:2080:ASP:HB2	1:A:2147:ILE:HG23	1.95	0.48
1:F:2026:PRO:O	1:F:2048:GLY:CA	2.61	0.48
1:B:2026:PRO:O	1:B:2048:GLY:CA	2.61	0.48
1:D:1999:SER:HB2	1:F:1974:THR:OG1	2.14	0.48
1:A:1976:THR:HG21	1:A:2045:ALA:HB1	1.96	0.48
1:B:1980:PHE:CD2	1:B:2022:VAL:HG11	2.49	0.48
1:B:2082:LYS:HA	1:B:2112:PRO:HD3	1.96	0.48
1:C:1963:LYS:HD3	1:C:2019:ASP:CG	2.35	0.47
1:B:2098:ARG:NH1	1:B:2098:ARG:HG3	2.28	0.47
1:C:2050:GLY:HA3	1:C:2085:ARG:HD3	1.94	0.47
1:E:2188:VAL:CG1	1:F:2004:GLY:O	2.62	0.47
1:D:2081:LEU:HD22	1:D:2087:VAL:HG11	1.96	0.47
1:E:2081:LEU:HD22	1:E:2087:VAL:HG11	1.95	0.47
1:F:1940:LEU:CD2	1:F:2057:LEU:CD2	2.92	0.47
1:C:2183:HIS:HD2	1:C:2184:PRO:HD2	1.79	0.47
1:C:2050:GLY:HA2	1:C:2085:ARG:HB3	1.96	0.47
1:A:2058:LEU:HD12	1:A:2059:ASP:N	2.30	0.47
1:D:1937:MET:O	1:D:1941:PHE:N	2.46	0.47
1:D:1980:PHE:CD2	1:D:2022:VAL:HG11	2.50	0.47
1:E:2136:LEU:O	1:E:2139:THR:HB	2.14	0.47
1:C:2183:HIS:CE1	1:C:2187:ARG:HB3	2.50	0.47
1:D:1940:LEU:CD2	1:D:2057:LEU:CD2	2.92	0.47
1:D:2088:HIS:CE1	1:D:2112:PRO:CG	2.98	0.47
1:A:2039:ARG:HH11	1:A:2039:ARG:CB	2.28	0.47
1:D:2129:PHE:CD2	1:D:2135:ALA:HB2	2.50	0.47
1:D:2082:LYS:HA	1:D:2112:PRO:HD3	1.97	0.46
1:E:2088:HIS:CE1	1:E:2112:PRO:HG2	2.51	0.46
1:F:1976:THR:HG21	1:F:2045:ALA:HB1	1.97	0.46
1:F:2159:GLU:O	1:F:2162:PHE:HB3	2.15	0.46
1:C:1937:MET:O	1:C:1941:PHE:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1976:THR:HG21	1:C:2045:ALA:HB1	1.97	0.46
1:E:1976:THR:HG21	1:E:2045:ALA:HB1	1.97	0.46
1:F:2001:VAL:C	1:F:2003:LYS:H	2.18	0.46
1:A:1980:PHE:CD2	1:A:2022:VAL:HG11	2.50	0.46
1:C:1976:THR:OG1	2:C:3226:CP:O	2.33	0.46
1:D:2060:ILE:CD1	1:D:2090:LEU:CD1	2.93	0.46
1:D:2211:MET:O	1:D:2215:MET:HG3	2.16	0.46
1:A:2060:ILE:CD1	1:A:2090:LEU:CD1	2.94	0.46
1:E:2183:HIS:HD2	1:E:2184:PRO:HD2	1.80	0.46
1:F:1937:MET:O	1:F:1941:PHE:N	2.46	0.46
1:A:2067:LEU:HD21	1:A:2180:VAL:HG12	1.96	0.46
1:B:1976:THR:HG21	1:B:2045:ALA:HB1	1.97	0.46
1:F:2060:ILE:CD1	1:F:2090:LEU:CD1	2.94	0.46
1:F:2082:LYS:HA	1:F:2112:PRO:HD3	1.96	0.46
1:B:2060:ILE:CD1	1:B:2090:LEU:CD1	2.94	0.46
1:B:2169:PRO:HD3	1:B:2192:SER:HB3	1.96	0.46
1:B:2211:MET:O	1:B:2215:MET:HG3	2.16	0.46
1:D:2167:LEU:HD11	1:D:2172:MET:CG	2.27	0.46
1:F:2058:LEU:HD12	1:F:2059:ASP:N	2.31	0.46
1:E:2214:ARG:O	1:E:2218:LEU:N	2.47	0.46
1:F:2047:ASP:CG	1:F:2049:VAL:HG22	2.35	0.46
1:C:2053:PRO:O	1:C:2057:LEU:HB2	2.16	0.46
1:C:2087:VAL:O	1:C:2091:ALA:CB	2.64	0.46
1:E:1980:PHE:CD2	1:E:2022:VAL:HG11	2.50	0.46
1:F:2066:GLU:CD	1:F:2205:ARG:HH12	2.19	0.46
1:A:1937:MET:O	1:A:1941:PHE:N	2.47	0.46
1:A:2020:VAL:CG1	1:A:2222:LEU:HD21	2.46	0.46
1:C:1956:SER:O	1:C:1957:LEU:HD23	2.16	0.46
1:C:2055:GLN:O	1:C:2058:LEU:HG	2.16	0.46
1:F:2139:THR:O	1:F:2139:THR:HG22	2.16	0.46
1:A:2133:GLU:O	1:A:2174:ARG:NH1	2.49	0.46
1:E:2082:LYS:HA	1:E:2112:PRO:HD3	1.98	0.46
1:E:2183:HIS:CE1	1:E:2187:ARG:HB3	2.51	0.46
1:F:2129:PHE:CD2	1:F:2135:ALA:HB2	2.50	0.46
1:F:2183:HIS:CE1	1:F:2187:ARG:HB3	2.51	0.46
1:A:2129:PHE:CG	1:A:2135:ALA:HB2	2.51	0.45
1:A:2136:LEU:N	1:A:2137:PRO:CD	2.79	0.45
1:B:2058:LEU:HD12	1:B:2059:ASP:N	2.31	0.45
1:D:1976:THR:HG21	1:D:2045:ALA:HB1	1.98	0.45
1:E:1940:LEU:CD2	1:E:2057:LEU:CD2	2.95	0.45
1:F:2087:VAL:O	1:F:2091:ALA:CB	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2020:VAL:CG1	1:F:2222:LEU:HD21	2.46	0.45
1:C:2211:MET:O	1:C:2215:MET:HG3	2.16	0.45
1:A:2002:GLN:HB2	1:C:1972:VAL:HG11	1.96	0.45
1:C:1945:HIS:O	1:C:1949:MET:HG2	2.17	0.45
1:D:1945:HIS:O	1:D:1949:MET:HG2	2.16	0.45
1:E:1978:SER:CB	1:F:2014:MET:HE1	2.46	0.45
1:A:2211:MET:O	1:A:2215:MET:HG3	2.15	0.45
1:C:1980:PHE:CD2	1:C:2022:VAL:HG11	2.51	0.45
1:D:1975:ARG:NH1	1:E:2013:THR:OG1	2.48	0.45
1:E:2087:VAL:O	1:E:2091:ALA:CB	2.64	0.45
1:E:2211:MET:O	1:E:2215:MET:HG3	2.16	0.45
1:F:2176:LYS:O	1:F:2200:ARG:NH1	2.46	0.45
1:A:2087:VAL:O	1:A:2091:ALA:CB	2.64	0.45
1:F:2211:MET:O	1:F:2215:MET:HG3	2.15	0.45
1:E:1945:HIS:O	1:E:1949:MET:HG2	2.17	0.45
1:A:2055:GLN:O	1:A:2058:LEU:HG	2.16	0.45
1:C:2058:LEU:HD12	1:C:2059:ASP:N	2.32	0.45
1:C:2139:THR:HG22	1:C:2139:THR:O	2.17	0.45
1:C:2166:ILE:HG23	1:C:2190:GLU:O	2.17	0.45
1:D:2020:VAL:CG1	1:D:2222:LEU:HD21	2.47	0.45
1:A:2082:LYS:HA	1:A:2112:PRO:HD3	1.98	0.45
1:E:2129:PHE:CD2	1:E:2135:ALA:HB2	2.52	0.45
1:B:1945:HIS:O	1:B:1949:MET:HG2	2.17	0.45
1:B:2047:ASP:CG	1:B:2049:VAL:HG22	2.37	0.45
1:C:2129:PHE:CD2	1:C:2135:ALA:HB2	2.52	0.45
1:E:2005:GLU:OE1	1:E:2009:ASP:HB3	2.16	0.45
1:A:1956:SER:O	1:A:1957:LEU:HD23	2.17	0.45
1:B:2055:GLN:O	1:B:2058:LEU:HG	2.17	0.45
1:D:2136:LEU:O	1:D:2139:THR:HB	2.17	0.45
1:B:2087:VAL:O	1:B:2091:ALA:CB	2.64	0.44
1:C:2050:GLY:CA	1:C:2085:ARG:CD	2.95	0.44
1:C:2214:ARG:O	1:C:2218:LEU:N	2.48	0.44
1:F:1956:SER:O	1:F:1957:LEU:HD23	2.17	0.44
1:F:2166:ILE:HG23	1:F:2190:GLU:O	2.17	0.44
1:B:1940:LEU:CD2	1:B:2057:LEU:CD2	2.95	0.44
1:E:1975:ARG:HB2	1:E:1975:ARG:CZ	2.48	0.44
1:E:2180:VAL:HG22	1:E:2202:ALA:HB3	1.99	0.44
1:F:1980:PHE:CD2	1:F:2022:VAL:HG11	2.52	0.44
1:F:2044:ASN:OD1	1:F:2045:ALA:N	2.50	0.44
1:C:1940:LEU:CD2	1:C:2057:LEU:HD21	2.48	0.44
1:C:2060:ILE:CD1	1:C:2090:LEU:CD1	2.96	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2060:ILE:CD1	1:E:2090:LEU:CD1	2.96	0.44
1:E:2168:THR:OG1	1:E:2171:ILE:HG12	2.17	0.44
1:E:1975:ARG:NH2	1:F:2005:GLU:OE2	2.50	0.44
1:C:2050:GLY:HA2	1:C:2085:ARG:HD2	1.98	0.44
1:D:2087:VAL:O	1:D:2091:ALA:CB	2.65	0.44
1:D:2147:ILE:HD12	1:D:2162:PHE:CD1	2.53	0.44
1:E:1949:MET:O	1:E:1953:LYS:CD	2.65	0.44
1:C:2168:THR:OG1	1:C:2171:ILE:HG12	2.17	0.44
1:D:1947:LEU:HD13	1:D:1987:LEU:HD21	1.98	0.44
1:F:1945:HIS:O	1:F:1949:MET:HG2	2.17	0.44
1:F:1947:LEU:HD13	1:F:1987:LEU:HD21	1.99	0.44
1:F:2136:LEU:N	1:F:2137:PRO:CD	2.81	0.44
1:D:2168:THR:HB	1:D:2169:PRO:CD	2.47	0.44
1:A:2044:ASN:OD1	1:A:2045:ALA:N	2.50	0.44
1:A:2060:ILE:CD1	1:A:2090:LEU:HD11	2.48	0.44
1:F:2060:ILE:CD1	1:F:2090:LEU:HD11	2.48	0.44
1:F:2136:LEU:CD1	1:F:2139:THR:HG21	2.47	0.44
1:B:1937:MET:O	1:B:1941:PHE:N	2.48	0.44
1:B:2090:LEU:HG	1:B:2094:LEU:HD22	1.99	0.44
1:B:2136:LEU:N	1:B:2137:PRO:CD	2.81	0.44
1:D:2214:ARG:O	1:D:2218:LEU:N	2.48	0.44
1:E:1956:SER:O	1:E:1957:LEU:HD23	2.17	0.44
1:F:1960:LEU:HD23	1:F:2224:ARG:HG3	2.00	0.44
1:F:2168:THR:OG1	1:F:2171:ILE:HG12	2.17	0.44
1:A:2005:GLU:OE2	1:C:1975:ARG:NH2	2.51	0.43
1:A:2142:LEU:O	1:A:2181:VAL:HG23	2.19	0.43
1:D:2060:ILE:CD1	1:D:2090:LEU:HD11	2.48	0.43
1:D:2129:PHE:CG	1:D:2135:ALA:HB2	2.52	0.43
1:A:2168:THR:OG1	1:A:2171:ILE:HG12	2.18	0.43
1:C:2044:ASN:OD1	1:C:2045:ALA:N	2.50	0.43
1:E:2025:HIS:O	1:E:2047:ASP:HA	2.19	0.43
1:F:2199:PRO:O	1:F:2201:ALA:N	2.50	0.43
1:A:1928:SER:OG	1:A:2051:GLU:OE2	2.36	0.43
1:A:2146:ARG:NH2	1:B:2004:GLY:O	2.50	0.43
1:C:1998:THR:HG22	1:C:1998:THR:O	2.19	0.43
1:D:2044:ASN:OD1	1:D:2045:ALA:N	2.51	0.43
1:D:2060:ILE:HD12	1:D:2090:LEU:CD1	2.48	0.43
1:E:2055:GLN:O	1:E:2058:LEU:HG	2.18	0.43
1:F:2014:MET:HA	1:F:2014:MET:HE3	1.99	0.43
1:B:2060:ILE:CD1	1:B:2090:LEU:HD11	2.48	0.43
1:C:2061:PHE:CZ	1:C:2065:GLU:CD	2.91	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2028:PRO:HA	1:E:2049:VAL:HG13	2.01	0.43
1:A:1947:LEU:HD13	1:A:1987:LEU:HD21	2.01	0.43
1:B:2020:VAL:CG1	1:B:2222:LEU:HD21	2.49	0.43
1:F:1970:TYR:N	1:F:1970:TYR:CD1	2.87	0.43
1:F:2055:GLN:O	1:F:2058:LEU:HG	2.18	0.43
1:A:2003:LYS:O	1:C:2146:ARG:NH1	2.36	0.43
1:A:2060:ILE:HD12	1:A:2090:LEU:CD1	2.48	0.43
1:B:2129:PHE:CD2	1:B:2135:ALA:HB2	2.54	0.43
1:D:1940:LEU:HD23	1:D:2057:LEU:CD2	2.49	0.43
1:D:1956:SER:O	1:D:1957:LEU:HD23	2.17	0.43
1:F:2005:GLU:HG2	1:F:2009:ASP:HB3	2.00	0.43
1:C:2136:LEU:CD1	1:C:2139:THR:HG21	2.49	0.43
1:E:1927:LEU:HA	1:E:2044:ASN:HB2	2.01	0.43
1:F:2090:LEU:HG	1:F:2094:LEU:HD22	1.99	0.43
1:B:1947:LEU:HD13	1:B:1987:LEU:HD21	1.99	0.43
1:A:1945:HIS:O	1:A:1949:MET:HG2	2.18	0.43
1:B:2088:HIS:NE2	1:B:2112:PRO:CG	2.82	0.43
1:B:2168:THR:OG1	1:B:2171:ILE:HG12	2.19	0.43
1:C:1927:LEU:HA	1:C:2044:ASN:HB2	2.01	0.43
1:C:2136:LEU:N	1:C:2137:PRO:CD	2.81	0.43
1:E:1947:LEU:HD13	1:E:1987:LEU:HD21	1.99	0.43
1:F:2124:THR:O	1:F:2125:LYS:O	2.36	0.43
1:F:2214:ARG:O	1:F:2218:LEU:N	2.47	0.43
1:A:1995:SER:HG	1:A:1998:THR:HG23	1.76	0.42
1:A:2039:ARG:HH11	1:A:2039:ARG:HB2	1.83	0.42
1:B:2060:ILE:HD12	1:B:2090:LEU:CD1	2.49	0.42
1:D:2136:LEU:HD12	1:D:2139:THR:HG21	2.01	0.42
1:F:2129:PHE:CG	1:F:2135:ALA:HB2	2.54	0.42
1:F:2142:LEU:O	1:F:2181:VAL:HG23	2.20	0.42
1:B:2044:ASN:OD1	1:B:2045:ALA:N	2.52	0.42
1:B:2120:ALA:HB2	1:B:2126:GLN:NE2	2.34	0.42
1:A:1980:PHE:CE1	1:A:2214:ARG:HG3	2.53	0.42
1:B:1956:SER:O	1:B:1957:LEU:HD23	2.18	0.42
1:B:1980:PHE:CE1	1:B:2214:ARG:HG3	2.54	0.42
1:D:2168:THR:OG1	1:D:2171:ILE:HG12	2.19	0.42
1:E:2020:VAL:CG1	1:E:2222:LEU:HD21	2.47	0.42
1:F:2025:HIS:O	1:F:2047:ASP:HA	2.18	0.42
1:A:1940:LEU:HD23	1:A:2057:LEU:CD2	2.47	0.42
1:A:2090:LEU:HG	1:A:2094:LEU:HD22	2.00	0.42
1:A:2098:ARG:NH1	1:A:2098:ARG:CG	2.82	0.42
1:B:2214:ARG:O	1:B:2218:LEU:N	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1947:LEU:HD13	1:C:1987:LEU:HD21	2.00	0.42
1:D:1970:TYR:CD1	1:D:1970:TYR:N	2.86	0.42
1:D:1975:ARG:HH22	1:E:2005:GLU:CD	2.23	0.42
1:F:2167:LEU:CD1	1:F:2181:VAL:HG21	2.49	0.42
1:C:2142:LEU:O	1:C:2181:VAL:HG23	2.19	0.42
1:D:2088:HIS:NE2	1:D:2112:PRO:CG	2.78	0.42
1:D:2142:LEU:O	1:D:2181:VAL:HG23	2.18	0.42
1:F:2005:GLU:CD	1:F:2009:ASP:HB3	2.39	0.42
1:A:1970:TYR:CD1	1:A:1970:TYR:N	2.88	0.42
1:A:1997:ALA:O	1:A:2002:GLN:NE2	2.52	0.42
1:C:2020:VAL:CG1	1:C:2222:LEU:HD21	2.47	0.42
1:C:2025:HIS:O	1:C:2047:ASP:HA	2.20	0.42
1:C:2066:GLU:CD	1:C:2205:ARG:NH2	2.70	0.42
1:D:2180:VAL:HG22	1:D:2202:ALA:HB3	2.01	0.42
1:E:2090:LEU:HG	1:E:2094:LEU:HD22	2.00	0.42
1:A:1960:LEU:HD23	1:A:2224:ARG:HG3	2.02	0.42
1:B:2025:HIS:O	1:B:2047:ASP:HA	2.20	0.42
1:B:1941:PHE:CZ	1:B:2060:ILE:CG2	3.02	0.42
1:B:2180:VAL:HG22	1:B:2202:ALA:HB3	2.01	0.42
1:C:2090:LEU:HG	1:C:2094:LEU:HD22	2.00	0.42
1:D:2058:LEU:HD23	1:D:2210:GLY:CA	2.42	0.42
1:E:2047:ASP:OD1	1:E:2050:GLY:HA2	2.20	0.42
1:F:2060:ILE:HD12	1:F:2090:LEU:CD1	2.50	0.42
1:B:1939:HIS:HA	1:B:1942:ASN:HD22	1.84	0.42
1:B:2213:ILE:CG1	1:B:2214:ARG:HD2	2.49	0.42
1:D:2028:PRO:HD3	3:D:4008:HOH:O	2.19	0.42
1:A:2102:ARG:NH2	1:A:2138:ASP:HB2	2.35	0.42
1:C:2065:GLU:O	1:E:1946:THR:OG1	2.32	0.42
1:C:2060:ILE:CD1	1:C:2090:LEU:HD11	2.50	0.42
1:C:2213:ILE:CG1	1:C:2214:ARG:HD2	2.50	0.42
1:D:2026:PRO:O	1:D:2048:GLY:CA	2.68	0.42
1:B:2120:ALA:CA	1:B:2126:GLN:HE22	2.32	0.41
1:B:2142:LEU:O	1:B:2181:VAL:HG23	2.19	0.41
1:F:2183:HIS:CD2	1:F:2184:PRO:HD2	2.54	0.41
1:C:2180:VAL:HG22	1:C:2202:ALA:HB3	2.02	0.41
1:D:1927:LEU:HA	1:D:2044:ASN:HB2	2.02	0.41
1:F:2005:GLU:HG2	1:F:2006:SER:N	2.35	0.41
1:F:2026:PRO:O	1:F:2048:GLY:HA3	2.20	0.41
1:A:2217:LEU:O	1:A:2218:LEU:C	2.57	0.41
1:B:2088:HIS:CE1	1:B:2112:PRO:CG	3.04	0.41
1:A:2183:HIS:CD2	1:A:2184:PRO:HD2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2066:GLU:CD	1:A:2205:ARG:NH2	2.73	0.41
1:C:1960:LEU:HD23	1:C:2224:ARG:HG3	2.02	0.41
1:E:2142:LEU:O	1:E:2181:VAL:HG23	2.20	0.41
1:F:2160:ALA:O	1:F:2163:GLY:N	2.54	0.41
1:B:1927:LEU:HA	1:B:2044:ASN:HB2	2.02	0.41
1:E:1980:PHE:CE1	1:E:2214:ARG:HG3	2.55	0.41
1:E:2044:ASN:OD1	1:E:2045:ALA:N	2.52	0.41
1:F:1927:LEU:HA	1:F:2044:ASN:HB2	2.02	0.41
1:B:2183:HIS:CE1	1:B:2187:ARG:CB	3.04	0.41
1:E:1959:ILE:HG23	1:E:2224:ARG:HB3	2.02	0.41
1:E:2060:ILE:CD1	1:E:2090:LEU:HD11	2.50	0.41
1:E:2183:HIS:CD2	1:E:2184:PRO:HD2	2.56	0.41
1:A:2148:GLN:O	1:A:2149:LYS:CB	2.68	0.41
1:D:2213:ILE:CG1	1:D:2214:ARG:HD2	2.50	0.41
1:E:1970:TYR:N	1:E:1970:TYR:CD1	2.88	0.41
1:A:2204:PHE:HB3	1:B:2039:ARG:HH21	1.86	0.41
1:A:2214:ARG:O	1:A:2218:LEU:N	2.49	0.41
1:E:2180:VAL:HG21	1:E:2202:ALA:CB	2.51	0.41
1:A:1927:LEU:HA	1:A:2044:ASN:HB2	2.02	0.41
1:B:2204:PHE:CZ	1:C:2012:GLN:HG2	2.56	0.41
1:D:2076:THR:HB	1:D:2142:LEU:HD12	2.02	0.41
1:E:2106:PRO:O	1:E:2108:SER:N	2.54	0.41
1:F:1980:PHE:CE1	1:F:2214:ARG:HG3	2.55	0.41
1:A:2180:VAL:HG22	1:A:2202:ALA:HB3	2.01	0.41
1:B:2180:VAL:HG21	1:B:2202:ALA:CB	2.51	0.41
1:B:2183:HIS:CD2	1:B:2184:PRO:HD2	2.54	0.41
1:B:2183:HIS:HE1	1:B:2187:ARG:CB	2.35	0.41
1:C:1965:MET:CE	1:C:1991:VAL:HG13	2.51	0.41
1:D:2183:HIS:CD2	1:D:2184:PRO:HD2	2.54	0.41
1:A:2164:GLN:C	1:A:2166:ILE:N	2.74	0.40
1:A:2180:VAL:CG2	1:A:2202:ALA:HB2	2.51	0.40
1:D:1976:THR:OG1	2:D:3226:CP:O1P	2.38	0.40
1:E:1939:HIS:HA	1:E:1942:ASN:HD22	1.85	0.40
1:F:2142:LEU:CD2	1:F:2167:LEU:HD11	2.42	0.40
1:B:2076:THR:HB	1:B:2142:LEU:HD12	2.03	0.40
1:C:2060:ILE:HD12	1:C:2090:LEU:CD1	2.50	0.40
1:F:1940:LEU:HD23	1:F:2057:LEU:CD2	2.49	0.40
1:C:2183:HIS:CD2	1:C:2184:PRO:HD2	2.55	0.40
1:B:1995:SER:HB3	1:B:1998:THR:OG1	2.21	0.40
1:C:2170:HIS:N	1:C:2170:HIS:ND1	2.68	0.40
1:D:2025:HIS:O	1:D:2047:ASP:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2136:LEU:N	1:D:2137:PRO:CD	2.85	0.40
1:F:2136:LEU:HD12	1:F:2139:THR:CG2	2.51	0.40
1:F:2185:MET:O	2:F:3226:CP:N	2.55	0.40
1:A:2000:SER:H	1:C:1974:THR:HG22	1.86	0.40
1:A:2180:VAL:HG21	1:A:2202:ALA:CB	2.51	0.40
1:B:1955:ARG:HD3	1:B:1956:SER:O	2.21	0.40
1:D:1965:MET:CE	1:D:1991:VAL:HG13	2.52	0.40
1:E:2139:THR:O	1:E:2139:THR:HG22	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1945:HIS:NE2	1:D:1945:HIS:CE1[1_454]	1.95	0.25

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	286/314 (91%)	247 (86%)	32 (11%)	7 (2%)	6	34
1	B	284/314 (90%)	251 (88%)	28 (10%)	5 (2%)	8	41
1	C	282/314 (90%)	247 (88%)	27 (10%)	8 (3%)	5	29
1	D	282/314 (90%)	241 (86%)	32 (11%)	9 (3%)	4	26
1	E	291/314 (93%)	247 (85%)	34 (12%)	10 (3%)	3	24
1	F	298/314 (95%)	249 (84%)	37 (12%)	12 (4%)	3	21
All	All	1723/1884 (92%)	1482 (86%)	190 (11%)	51 (3%)	4	28

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2149	LYS
1	D	2147	ILE
1	D	2148	GLN
1	F	1916	PRO
1	F	2125	LYS
1	F	2154	SER
1	A	2084	GLY
1	A	2147	ILE
1	A	2148	GLN
1	C	1954	GLU
1	C	2084	GLY
1	C	2147	ILE
1	D	2000	SER
1	D	2084	GLY
1	E	1954	GLU
1	E	2084	GLY
1	E	2188	VAL
1	F	2084	GLY
1	F	2151	ARG
1	F	2153	GLY
1	F	2159	GLU
1	A	1993	SER
1	A	2188	VAL
1	B	2084	GLY
1	B	2172	MET
1	C	2188	VAL
1	E	2148	GLN
1	F	2148	GLN
1	F	2188	VAL
1	B	2188	VAL
1	C	1993	SER
1	C	2148	GLN
1	D	2150	GLU
1	D	2188	VAL
1	E	2107	PRO
1	E	2124	THR
1	A	2172	MET
1	B	1954	GLU
1	C	2172	MET
1	D	1993	SER
1	D	2107	PRO
1	E	1993	SER
1	E	2172	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	2199	PRO
1	F	1918	LEU
1	B	1922	VAL
1	C	1922	VAL
1	D	1922	VAL
1	E	1922	VAL
1	F	1922	VAL
1	F	2004	GLY

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	226/268 (84%)	201 (89%)	25 (11%)	6	25
1	B	220/268 (82%)	192 (87%)	28 (13%)	4	20
1	C	221/268 (82%)	199 (90%)	22 (10%)	7	30
1	D	224/268 (84%)	202 (90%)	22 (10%)	8	31
1	E	218/268 (81%)	193 (88%)	25 (12%)	5	24
1	F	223/268 (83%)	202 (91%)	21 (9%)	8	33
All	All	1332/1608 (83%)	1189 (89%)	143 (11%)	6	27

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1929	VAL
1	A	1938	SER
1	A	1955	ARG
1	A	1978	SER
1	A	2006	SER
1	A	2009	ASP
1	A	2010	SER
1	A	2025	HIS
1	A	2033	LEU
1	A	2036	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2039	ARG
1	A	2062	THR
1	A	2064	ARG
1	A	2067	LEU
1	A	2074	THR
1	A	2087	VAL
1	A	2089	SER
1	A	2094	LEU
1	A	2100	SER
1	A	2108	SER
1	A	2124	THR
1	A	2139	THR
1	A	2146	ARG
1	A	2188	VAL
1	A	2225	PHE
1	B	1929	VAL
1	B	1938	SER
1	B	1954	GLU
1	B	1971	GLU
1	B	1978	SER
1	B	1995	SER
1	B	2006	SER
1	B	2009	ASP
1	B	2010	SER
1	B	2025	HIS
1	B	2033	LEU
1	B	2062	THR
1	B	2064	ARG
1	B	2087	VAL
1	B	2089	SER
1	B	2094	LEU
1	B	2098	ARG
1	B	2100	SER
1	B	2108	SER
1	B	2114	THR
1	B	2115	VAL
1	B	2124	THR
1	B	2126	GLN
1	B	2134	GLU
1	B	2138	ASP
1	B	2139	THR
1	B	2188	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2225	PHE
1	C	1929	VAL
1	C	1953	LYS
1	C	1955	ARG
1	C	1961	LYS
1	C	1978	SER
1	C	1998	THR
1	C	2006	SER
1	C	2009	ASP
1	C	2010	SER
1	C	2025	HIS
1	C	2033	LEU
1	C	2039	ARG
1	C	2062	THR
1	C	2064	ARG
1	C	2089	SER
1	C	2094	LEU
1	C	2095	THR
1	C	2138	ASP
1	C	2139	THR
1	C	2174	ARG
1	C	2188	VAL
1	C	2225	PHE
1	D	1929	VAL
1	D	1955	ARG
1	D	1974	THR
1	D	1978	SER
1	D	1998	THR
1	D	2006	SER
1	D	2009	ASP
1	D	2010	SER
1	D	2025	HIS
1	D	2062	THR
1	D	2087	VAL
1	D	2089	SER
1	D	2100	SER
1	D	2108	SER
1	D	2134	GLU
1	D	2139	THR
1	D	2167	LEU
1	D	2174	ARG
1	D	2177	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2188	VAL
1	D	2224	ARG
1	D	2225	PHE
1	E	1919	HIS
1	E	1929	VAL
1	E	1953	LYS
1	E	1955	ARG
1	E	1974	THR
1	E	1978	SER
1	E	2006	SER
1	E	2009	ASP
1	E	2010	SER
1	E	2025	HIS
1	E	2033	LEU
1	E	2062	THR
1	E	2064	ARG
1	E	2087	VAL
1	E	2089	SER
1	E	2094	LEU
1	E	2098	ARG
1	E	2100	SER
1	E	2139	THR
1	E	2162	PHE
1	E	2174	ARG
1	E	2188	VAL
1	E	2189	ASN
1	E	2224	ARG
1	E	2225	PHE
1	F	1929	VAL
1	F	1974	THR
1	F	1978	SER
1	F	2006	SER
1	F	2009	ASP
1	F	2010	SER
1	F	2025	HIS
1	F	2039	ARG
1	F	2062	THR
1	F	2087	VAL
1	F	2088	HIS
1	F	2089	SER
1	F	2094	LEU
1	F	2100	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	2138	ASP
1	F	2139	THR
1	F	2167	LEU
1	F	2170	HIS
1	F	2188	VAL
1	F	2218	LEU
1	F	2225	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1931	GLN
1	A	1942	ASN
1	A	2002	GLN
1	A	2183	HIS
1	B	1942	ASN
1	B	1945	HIS
1	B	2126	GLN
1	B	2183	HIS
1	C	2183	HIS
1	D	1936	GLN
1	D	1942	ASN
1	D	2126	GLN
1	D	2183	HIS
1	E	2183	HIS
1	E	2189	ASN
1	F	1936	GLN
1	F	1942	ASN
1	F	1945	HIS
1	F	2083	HIS
1	F	2183	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CP	F	3226	-	6,7,7	1.09	1 (16%)	7,10,10	1.43	2 (28%)
2	CP	D	3226	-	6,7,7	0.77	0	7,10,10	2.13	5 (71%)
2	CP	A	3226	-	6,7,7	1.40	1 (16%)	7,10,10	0.93	0
2	CP	E	3226	-	6,7,7	1.06	0	7,10,10	1.52	1 (14%)
2	CP	C	3226	-	6,7,7	1.29	1 (16%)	7,10,10	1.83	1 (14%)
2	CP	B	3226	-	6,7,7	1.12	0	7,10,10	1.62	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CP	F	3226	-	-	0/3/5/5	-
2	CP	D	3226	-	-	0/3/5/5	-
2	CP	A	3226	-	-	0/3/5/5	-
2	CP	E	3226	-	-	0/3/5/5	-
2	CP	C	3226	-	-	0/3/5/5	-
2	CP	B	3226	-	-	0/3/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3226	CP	P-O4P	2.98	1.63	1.59
2	C	3226	CP	P-O4P	2.42	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3226	CP	P-O4P	2.29	1.62	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3226	CP	O-C-N	-3.95	119.00	125.51
2	B	3226	CP	O-C-N	-2.87	120.77	125.51
2	E	3226	CP	O3P-P-O2P	2.81	118.38	107.64
2	D	3226	CP	O3P-P-O1P	2.62	120.94	110.68
2	D	3226	CP	O3P-P-O2P	2.45	117.00	107.64
2	D	3226	CP	O-C-N	-2.32	121.69	125.51
2	B	3226	CP	O3P-P-O2P	2.29	116.39	107.64
2	D	3226	CP	O3P-P-O4P	-2.22	98.49	105.25
2	F	3226	CP	O-C-N	-2.22	121.85	125.51
2	F	3226	CP	O3P-P-O2P	2.11	115.71	107.64
2	D	3226	CP	O4P-P-O1P	-2.07	101.97	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3226	CP	4	0
2	D	3226	CP	4	0
2	E	3226	CP	1	0
2	C	3226	CP	2	0

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	292/314 (92%)	0.37	27 (9%) 9 5	23, 51, 80, 94	0
1	B	288/314 (91%)	0.38	24 (8%) 11 6	24, 53, 83, 100	0
1	C	288/314 (91%)	0.45	30 (10%) 6 4	22, 47, 72, 88	0
1	D	292/314 (92%)	0.49	35 (11%) 4 2	17, 49, 82, 110	0
1	E	299/314 (95%)	0.29	20 (6%) 17 10	26, 49, 74, 90	0
1	F	304/314 (96%)	0.49	30 (9%) 7 4	19, 49, 75, 98	0
All	All	1763/1884 (93%)	0.41	166 (9%) 8 4	17, 49, 78, 110	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2074	THR	9.0
1	F	2198	ASP	7.0
1	D	2089	SER	6.4
1	C	1974	THR	5.8
1	D	2121	SER	5.5
1	E	2164	GLN	5.2
1	C	2145	THR	5.2
1	F	2124	THR	5.1
1	E	2206	GLN	5.0
1	E	1977	SER	5.0
1	C	1977	SER	4.9
1	C	1944	ALA	4.9
1	E	2191	ILE	4.9
1	E	2192	SER	4.7
1	F	2130	GLU	4.6
1	F	2144	MET	4.5
1	B	2196	ASP	4.5
1	F	2145	THR	4.3
1	F	1993	SER	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	2018	ALA	4.2
1	A	2086	THR	4.0
1	C	2095	THR	4.0
1	F	2203	TYR	3.9
1	F	1935	ASP	3.9
1	C	2028	PRO	3.9
1	B	2106	PRO	3.8
1	C	2017	TYR	3.7
1	B	2181	VAL	3.7
1	C	1978	SER	3.7
1	B	1951	VAL	3.5
1	B	2145	THR	3.5
1	F	2199	PRO	3.5
1	A	2169	PRO	3.5
1	F	2104	VAL	3.4
1	D	2057	LEU	3.4
1	E	1959	ILE	3.4
1	D	2081	LEU	3.4
1	F	2123	GLY	3.4
1	E	2089	SER	3.3
1	E	1952	GLN	3.3
1	B	2097	TYR	3.3
1	D	2101	LEU	3.3
1	F	2161	CYS	3.3
1	D	2212	TYR	3.2
1	C	2027	GLN	3.2
1	E	2167	LEU	3.2
1	F	2056	ALA	3.2
1	F	2222	LEU	3.2
1	A	2004	GLY	3.2
1	E	2138	ASP	3.2
1	A	1958	ASP	3.1
1	D	2047	ASP	3.1
1	D	2214	ARG	3.1
1	D	2093	LEU	3.1
1	D	2048	GLY	3.1
1	C	2021	VAL	3.1
1	F	2018	ALA	3.1
1	B	2119	VAL	3.1
1	B	2089	SER	3.0
1	C	2080	ASP	3.0
1	F	2141	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2018	ALA	3.0
1	D	2120	ALA	3.0
1	C	2161	CYS	3.0
1	F	2135	ALA	2.9
1	F	2202	ALA	2.9
1	D	2204	PHE	2.9
1	A	1924	GLN	2.9
1	A	2193	VAL	2.9
1	B	2082	LYS	2.9
1	F	1938	SER	2.9
1	B	2194	GLU	2.9
1	A	2042	VAL	2.8
1	D	2123	GLY	2.8
1	C	2015	SER	2.8
1	C	2183	HIS	2.8
1	F	2223	GLY	2.8
1	F	2160	ALA	2.8
1	A	2053	PRO	2.8
1	C	1973	SER	2.8
1	D	2128	GLU	2.8
1	C	2136	LEU	2.7
1	D	1981	ALA	2.7
1	F	2016	CYS	2.7
1	E	2188	VAL	2.7
1	D	2068	GLY	2.7
1	F	2072	GLY	2.7
1	F	2095	THR	2.7
1	D	2225	PHE	2.7
1	C	1938	SER	2.6
1	E	2145	THR	2.6
1	B	2103	TYR	2.6
1	C	1981	ALA	2.6
1	A	2008	ALA	2.6
1	D	2027	GLN	2.6
1	A	2079	GLY	2.6
1	C	2132	ILE	2.6
1	E	2163	GLY	2.5
1	B	2058	LEU	2.5
1	A	2196	ASP	2.5
1	C	1980	PHE	2.5
1	C	1956	SER	2.5
1	B	1939	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	2190	GLU	2.5
1	B	2038	CYS	2.5
1	E	2130	GLU	2.5
1	A	2074	THR	2.5
1	D	2072	GLY	2.5
1	B	2197	SER	2.5
1	F	2055	GLN	2.5
1	C	2005	GLU	2.5
1	B	2186	PRO	2.4
1	C	1990	ALA	2.4
1	B	2143	TYR	2.4
1	D	2210	GLY	2.4
1	D	2086	THR	2.4
1	F	2113	PRO	2.4
1	A	2089	SER	2.4
1	A	2113	PRO	2.4
1	D	2132	ILE	2.4
1	F	2173	THR	2.4
1	E	2125	LYS	2.4
1	D	1946	THR	2.4
1	F	2213	ILE	2.4
1	D	2169	PRO	2.3
1	A	2037	HIS	2.3
1	A	1966	ALA	2.3
1	A	2005	GLU	2.3
1	E	2139	THR	2.3
1	E	2097	TYR	2.3
1	A	2104	VAL	2.3
1	D	2092	CYS	2.3
1	D	2213	ILE	2.3
1	D	1983	ALA	2.3
1	C	2056	ALA	2.2
1	B	2178	LYS	2.2
1	A	2182	MET	2.2
1	C	2204	PHE	2.2
1	D	1951	VAL	2.2
1	D	1931	GLN	2.2
1	A	2223	GLY	2.2
1	D	2202	ALA	2.2
1	E	2029	GLY	2.2
1	D	2045	ALA	2.2
1	D	1980	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2096	GLN	2.2
1	A	2006	SER	2.2
1	C	1936	GLN	2.2
1	A	1988	GLY	2.2
1	A	2183	HIS	2.2
1	A	1973	SER	2.1
1	A	2000	SER	2.1
1	B	2015	SER	2.1
1	C	2179	MET	2.1
1	A	1986	ARG	2.1
1	F	2172	MET	2.1
1	C	2092	CYS	2.1
1	D	2071	ASN	2.1
1	C	2055	GLN	2.1
1	D	2069	THR	2.1
1	D	2127	GLU	2.0
1	B	2132	ILE	2.0
1	A	2132	ILE	2.0
1	B	1952	GLN	2.0
1	E	2216	ALA	2.0
1	B	2101	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CP	A	3226	8/8	0.84	0.24	34,49,61,64	0
2	CP	F	3226	8/8	0.92	0.17	43,46,52,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CP	C	3226	8/8	0.93	0.16	41,44,49,51	0
2	CP	E	3226	8/8	0.94	0.15	28,32,34,35	0
2	CP	D	3226	8/8	0.94	0.17	25,29,32,32	0
2	CP	B	3226	8/8	0.96	0.14	31,33,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.