



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 1X8M / pdb_00001x8m
Title : X-ray structure of pectin degrading enzyme 5-keto 4-deoxyuronate isomerase from Escherichia coli
Authors : Fedorov, A.A.; Fedorov, E.V.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-08-18
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

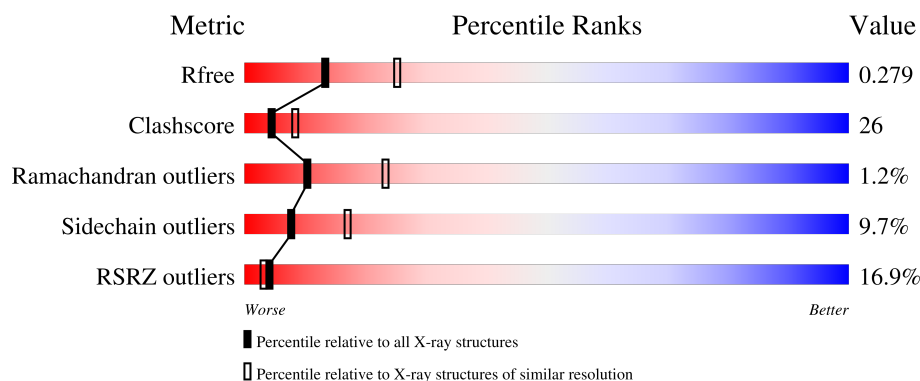
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	288	11% 52% 31% 6% 10%
1	B	288	14% 55% 29% 5% 10%
1	C	288	12% 50% 33% 6% 10%
1	D	288	16% 54% 28% 7% 10%
1	E	288	22% 52% 30% 7% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	288	16% 55% 28% 6% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12126 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 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2021	1284	341	383	13			
1	B	259	Total	C	N	O	S	0	0	0
			2021	1284	341	383	13			
1	C	259	Total	C	N	O	S	0	0	0
			2021	1284	341	383	13			
1	D	259	Total	C	N	O	S	0	0	0
			2021	1284	341	383	13			
1	E	259	Total	C	N	O	S	0	0	0
			2021	1284	341	383	13			
1	F	259	Total	C	N	O	S	0	0	0
			2021	1284	341	383	13			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	MET	-	cloning artifact	UNP Q46938
A	1002	SER	-	cloning artifact	UNP Q46938
A	1003	LEU	-	cloning artifact	UNP Q46938
A	1281	GLU	-	expression tag	UNP Q46938
A	1282	GLY	-	expression tag	UNP Q46938
A	1283	HIS	-	expression tag	UNP Q46938
A	1284	HIS	-	expression tag	UNP Q46938
A	1285	HIS	-	expression tag	UNP Q46938
A	1286	HIS	-	expression tag	UNP Q46938
A	1287	HIS	-	expression tag	UNP Q46938
A	1288	HIS	-	expression tag	UNP Q46938
B	2001	MET	-	cloning artifact	UNP Q46938
B	2002	SER	-	cloning artifact	UNP Q46938
B	2003	LEU	-	cloning artifact	UNP Q46938
B	2281	GLU	-	expression tag	UNP Q46938
B	2282	GLY	-	expression tag	UNP Q46938
B	2283	HIS	-	expression tag	UNP Q46938

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2284	HIS	-	expression tag	UNP Q46938
B	2285	HIS	-	expression tag	UNP Q46938
B	2286	HIS	-	expression tag	UNP Q46938
B	2287	HIS	-	expression tag	UNP Q46938
B	2288	HIS	-	expression tag	UNP Q46938
C	3001	MET	-	cloning artifact	UNP Q46938
C	3002	SER	-	cloning artifact	UNP Q46938
C	3003	LEU	-	cloning artifact	UNP Q46938
C	3281	GLU	-	expression tag	UNP Q46938
C	3282	GLY	-	expression tag	UNP Q46938
C	3283	HIS	-	expression tag	UNP Q46938
C	3284	HIS	-	expression tag	UNP Q46938
C	3285	HIS	-	expression tag	UNP Q46938
C	3286	HIS	-	expression tag	UNP Q46938
C	3287	HIS	-	expression tag	UNP Q46938
C	3288	HIS	-	expression tag	UNP Q46938
D	4001	MET	-	cloning artifact	UNP Q46938
D	4002	SER	-	cloning artifact	UNP Q46938
D	4003	LEU	-	cloning artifact	UNP Q46938
D	4281	GLU	-	expression tag	UNP Q46938
D	4282	GLY	-	expression tag	UNP Q46938
D	4283	HIS	-	expression tag	UNP Q46938
D	4284	HIS	-	expression tag	UNP Q46938
D	4285	HIS	-	expression tag	UNP Q46938
D	4286	HIS	-	expression tag	UNP Q46938
D	4287	HIS	-	expression tag	UNP Q46938
D	4288	HIS	-	expression tag	UNP Q46938
E	5001	MET	-	cloning artifact	UNP Q46938
E	5002	SER	-	cloning artifact	UNP Q46938
E	5003	LEU	-	cloning artifact	UNP Q46938
E	5281	GLU	-	expression tag	UNP Q46938
E	5282	GLY	-	expression tag	UNP Q46938
E	5283	HIS	-	expression tag	UNP Q46938
E	5284	HIS	-	expression tag	UNP Q46938
E	5285	HIS	-	expression tag	UNP Q46938
E	5286	HIS	-	expression tag	UNP Q46938
E	5287	HIS	-	expression tag	UNP Q46938
E	5288	HIS	-	expression tag	UNP Q46938
F	6001	MET	-	cloning artifact	UNP Q46938
F	6002	SER	-	cloning artifact	UNP Q46938
F	6003	LEU	-	cloning artifact	UNP Q46938
F	6281	GLU	-	expression tag	UNP Q46938

Continued on next page...

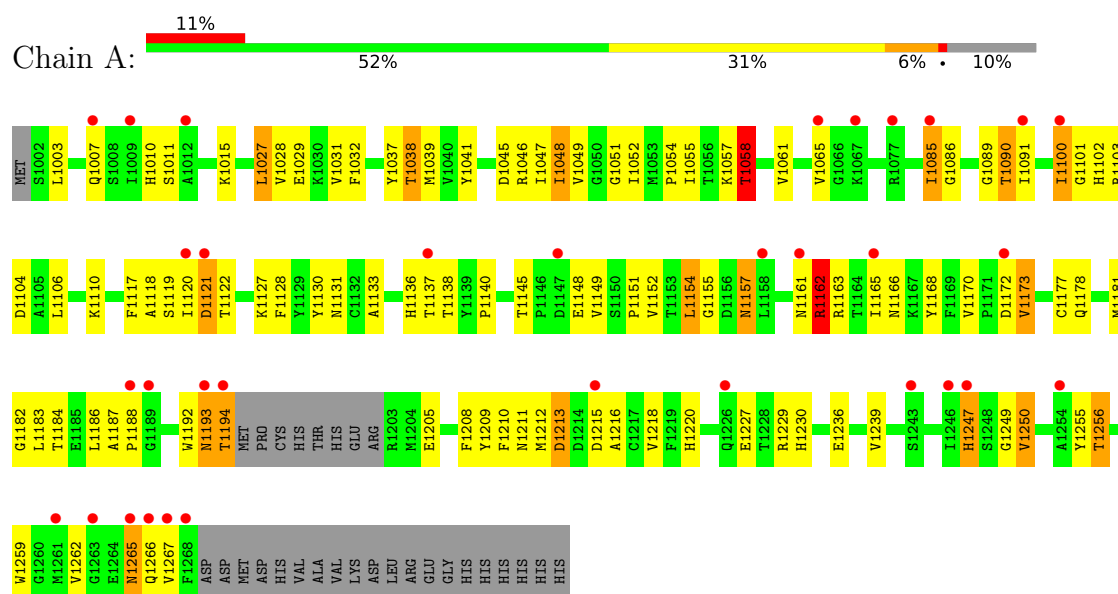
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	6282	GLY	-	expression tag	UNP Q46938
F	6283	HIS	-	expression tag	UNP Q46938
F	6284	HIS	-	expression tag	UNP Q46938
F	6285	HIS	-	expression tag	UNP Q46938
F	6286	HIS	-	expression tag	UNP Q46938
F	6287	HIS	-	expression tag	UNP Q46938
F	6288	HIS	-	expression tag	UNP Q46938

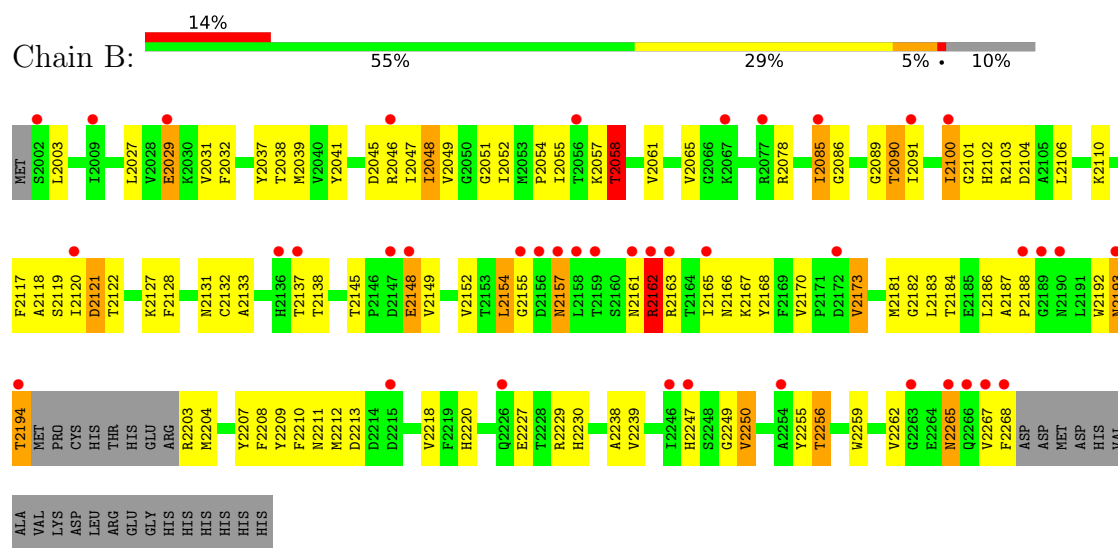
3 Residue-property plots

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.

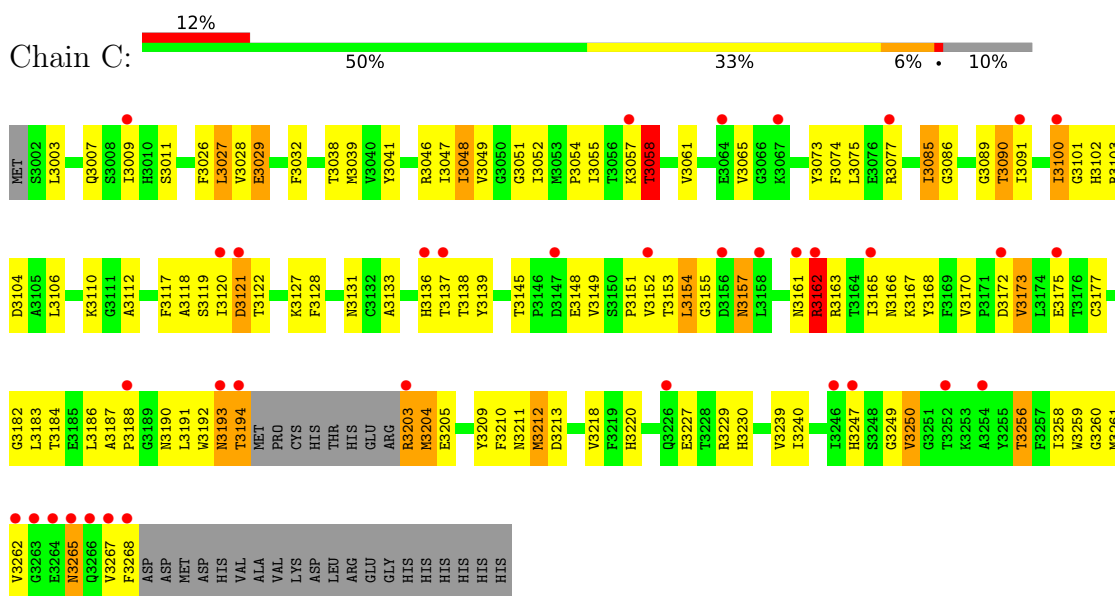
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



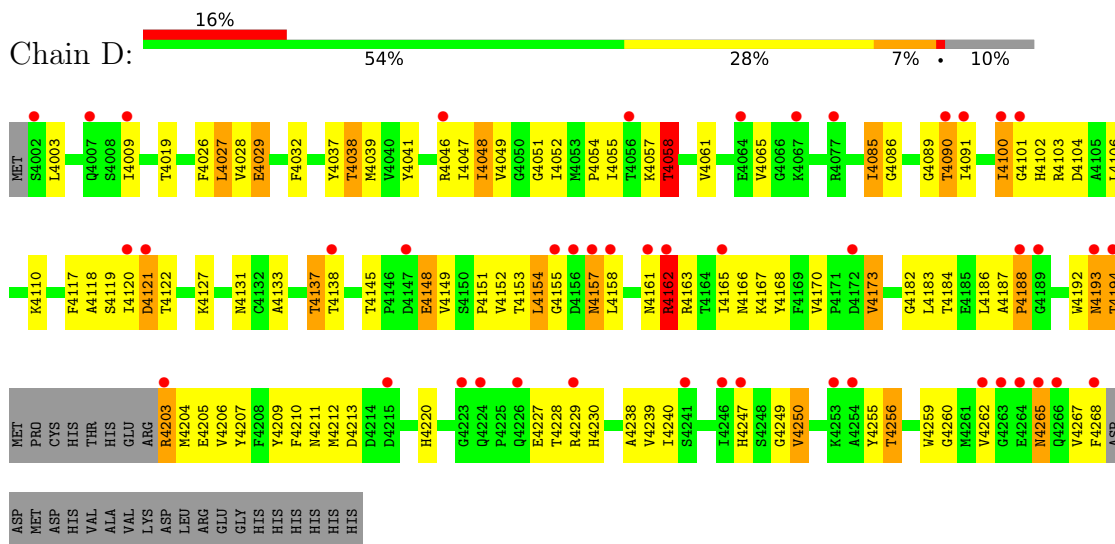
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



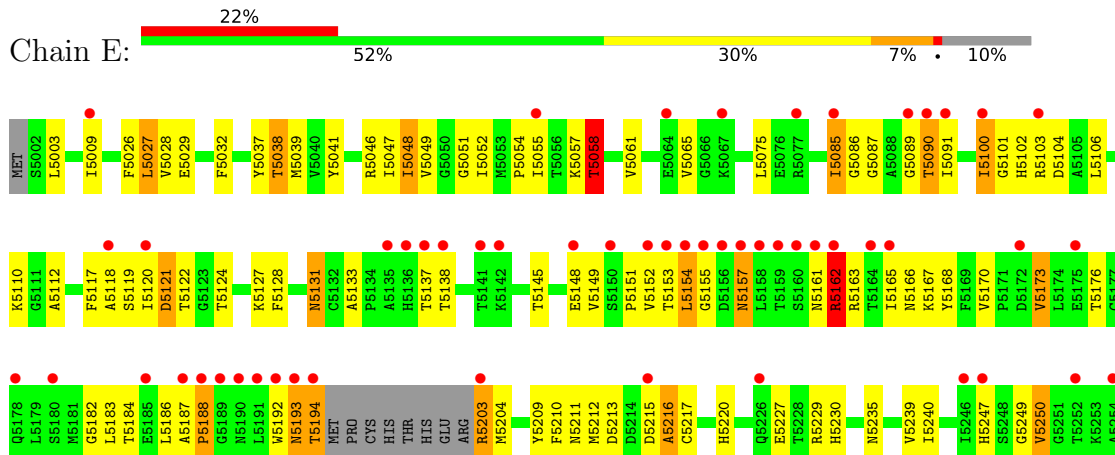
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase

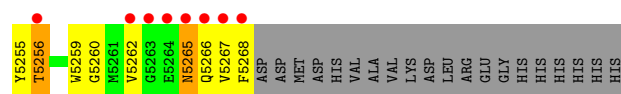


- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase

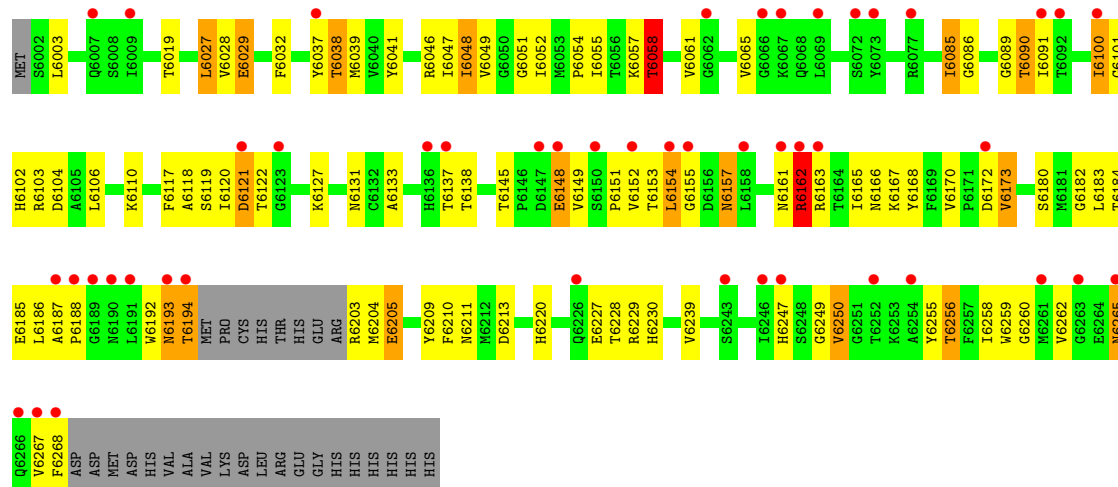


- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase





- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	101.01Å 101.01Å 179.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.60 25.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.00-2.60) 99.0 (25.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.280 0.254 , 0.279	Depositor DCC
R_{free} test set	3176 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.037 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12126	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4544e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/2067	0.98	3/2806 (0.1%)
1	B	0.53	0/2067	0.98	3/2806 (0.1%)
1	C	0.53	0/2067	0.97	3/2806 (0.1%)
1	D	0.53	0/2067	0.99	3/2806 (0.1%)
1	E	0.53	0/2067	0.99	3/2806 (0.1%)
1	F	0.51	0/2067	0.98	4/2806 (0.1%)
All	All	0.52	0/12402	0.98	19/16836 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	6265	ASN	N-CA-C	6.35	122.10	113.21
1	B	2265	ASN	N-CA-C	6.34	122.09	113.21
1	A	1265	ASN	N-CA-C	6.23	121.93	113.21
1	B	2058	THR	N-CA-C	-6.19	100.06	109.85
1	D	4265	ASN	N-CA-C	6.17	121.85	113.21
1	E	5265	ASN	N-CA-C	6.07	121.70	113.21
1	C	3265	ASN	N-CA-C	5.99	121.60	113.21
1	E	5058	THR	N-CA-C	-5.87	100.58	109.85
1	A	1058	THR	N-CA-C	-5.77	100.73	109.85
1	F	6058	THR	N-CA-C	-5.72	100.81	109.85
1	D	4058	THR	N-CA-C	-5.55	101.08	109.85
1	C	3058	THR	N-CA-C	-5.48	101.20	109.85
1	C	3029	GLU	N-CA-C	5.43	116.88	111.07
1	F	6029	GLU	N-CA-C	5.25	116.68	111.07
1	E	5131	ASN	N-CA-C	-5.22	100.52	109.24
1	D	4029	GLU	N-CA-C	5.19	116.62	111.07
1	A	1029	GLU	N-CA-C	5.12	116.55	111.07
1	F	6131	ASN	N-CA-C	-5.11	100.72	109.24
1	B	2029	GLU	N-CA-C	5.06	116.49	111.07

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	2021	0	1972	117	0
1	B	2021	0	1972	98	0
1	C	2021	0	1972	115	0
1	D	2021	0	1972	116	0
1	E	2021	0	1972	107	0
1	F	2021	0	1972	107	0
All	All	12126	0	11832	630	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 26.

All (630) 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:E:5163:ARG:HB3	1:E:5186:LEU:HD23	1.36	1.08
1:C:3163:ARG:HB3	1:C:3186:LEU:HD23	1.37	1.07
1:D:4163:ARG:HB3	1:D:4186:LEU:HD23	1.37	1.07
1:A:1163:ARG:HB3	1:A:1186:LEU:HD23	1.36	1.05
1:F:6163:ARG:HB3	1:F:6186:LEU:HD23	1.38	1.04
1:C:3175:GLU:OE1	1:D:4153:THR:HB	1.59	1.02
1:F:6039:MET:HG3	1:F:6048:ILE:HD13	1.42	1.02
1:B:2163:ARG:HB3	1:B:2186:LEU:HD23	1.38	1.01
1:E:5047:ILE:HD11	1:E:5262:VAL:HG11	1.38	1.00
1:E:5061:VAL:HG23	1:E:5065:VAL:HG21	1.44	0.98
1:D:4047:ILE:HD11	1:D:4262:VAL:HG11	1.45	0.98
1:A:1061:VAL:HG23	1:A:1065:VAL:HG21	1.46	0.97
1:B:2039:MET:HG3	1:B:2048:ILE:HD13	1.45	0.97
1:B:2061:VAL:HG23	1:B:2065:VAL:HG21	1.46	0.97
1:E:5039:MET:HG3	1:E:5048:ILE:HD13	1.45	0.97
1:C:3061:VAL:HG23	1:C:3065:VAL:HG21	1.46	0.96
1:D:4039:MET:HG3	1:D:4048:ILE:HD13	1.45	0.96
1:A:1039:MET:HG3	1:A:1048:ILE:HD13	1.44	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6061:VAL:HG23	1:F:6065:VAL:HG21	1.49	0.95
1:D:4061:VAL:HG23	1:D:4065:VAL:HG21	1.47	0.92
1:C:3039:MET:HG3	1:C:3048:ILE:HD13	1.50	0.91
1:A:1011:SER:H	1:C:3007:GLN:HE22	1.08	0.90
1:A:1136:HIS:HB2	1:C:3136:HIS:HB2	1.52	0.90
1:C:3091:ILE:HD13	1:C:3106:LEU:HD23	1.55	0.86
1:F:6091:ILE:HD13	1:F:6106:LEU:HD23	1.56	0.86
1:E:5211:ASN:HB3	1:E:5256:THR:HG23	1.59	0.85
1:A:1091:ILE:HD13	1:A:1106:LEU:HD23	1.59	0.84
1:C:3047:ILE:HD11	1:C:3262:VAL:HG11	1.59	0.84
1:E:5091:ILE:HD13	1:E:5106:LEU:HD23	1.58	0.83
1:A:1136:HIS:H	1:C:3136:HIS:HD2	1.26	0.82
1:A:1047:ILE:HD11	1:A:1262:VAL:HG11	1.59	0.82
1:D:4091:ILE:HD13	1:D:4106:LEU:HD23	1.59	0.82
1:B:2091:ILE:HD13	1:B:2106:LEU:HD23	1.60	0.82
1:A:1011:SER:H	1:C:3007:GLN:NE2	1.80	0.80
1:A:1055:ILE:O	1:A:1122:THR:HG22	1.82	0.80
1:B:2157:ASN:HD22	1:B:2157:ASN:N	1.79	0.80
1:F:6211:ASN:HB3	1:F:6256:THR:HG23	1.62	0.80
1:A:1157:ASN:HD22	1:A:1157:ASN:N	1.80	0.79
1:F:6055:ILE:O	1:F:6122:THR:HG22	1.82	0.78
1:C:3157:ASN:HD22	1:C:3157:ASN:N	1.81	0.78
1:B:2055:ILE:O	1:B:2122:THR:HG22	1.83	0.77
1:F:6157:ASN:HD22	1:F:6157:ASN:N	1.81	0.77
1:E:5055:ILE:O	1:E:5122:THR:HG22	1.83	0.77
1:D:4055:ILE:O	1:D:4122:THR:HG22	1.84	0.77
1:B:2211:ASN:HB3	1:B:2256:THR:HG23	1.65	0.77
1:C:3055:ILE:O	1:C:3122:THR:HG22	1.84	0.76
1:D:4211:ASN:HB3	1:D:4256:THR:HG23	1.68	0.76
1:E:5192:TRP:CZ3	1:E:5250:VAL:HG22	2.22	0.75
1:C:3139:TYR:CE2	1:D:4162:ARG:NH2	2.55	0.75
1:A:1192:TRP:CZ3	1:A:1250:VAL:HG22	2.21	0.75
1:C:3211:ASN:HB3	1:C:3256:THR:HG23	1.66	0.74
1:B:2047:ILE:HD11	1:B:2262:VAL:HG11	1.69	0.74
1:B:2209:TYR:OH	1:B:2220:HIS:HD2	1.71	0.73
1:E:5157:ASN:HD22	1:E:5157:ASN:N	1.83	0.73
1:D:4209:TYR:OH	1:D:4220:HIS:HD2	1.72	0.73
1:E:5211:ASN:HD22	1:E:5256:THR:HG21	1.55	0.72
1:C:3161:ASN:HB3	1:C:3163:ARG:NH1	2.04	0.72
1:D:4161:ASN:HB3	1:D:4163:ARG:NH1	2.04	0.72
1:C:3209:TYR:OH	1:C:3220:HIS:HD2	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4230:HIS:HE1	1:F:6228:THR:OG1	1.73	0.71
1:E:5161:ASN:HB3	1:E:5163:ARG:NH1	2.05	0.71
1:E:5102:HIS:ND1	1:E:5103:ARG:HG2	2.06	0.71
1:A:1211:ASN:HB3	1:A:1256:THR:HG23	1.73	0.71
1:D:4157:ASN:HD22	1:D:4157:ASN:N	1.89	0.71
1:E:5193:ASN:HD21	1:E:5249:GLY:H	1.39	0.71
1:E:5209:TYR:OH	1:E:5220:HIS:HD2	1.74	0.71
1:D:4101:GLY:O	1:D:4104:ASP:HB2	1.92	0.70
1:A:1193:ASN:HD21	1:A:1249:GLY:H	1.40	0.69
1:C:3102:HIS:ND1	1:C:3103:ARG:HG2	2.08	0.69
1:F:6161:ASN:HB3	1:F:6163:ARG:NH1	2.08	0.69
1:D:4192:TRP:CZ3	1:D:4250:VAL:HG22	2.28	0.69
1:D:4204:MET:HE1	1:D:4240:ILE:HG23	1.74	0.69
1:E:5039:MET:HG3	1:E:5048:ILE:CD1	2.22	0.69
1:B:2161:ASN:HB3	1:B:2163:ARG:NH1	2.09	0.68
1:E:5101:GLY:O	1:E:5104:ASP:HB2	1.93	0.68
1:A:1161:ASN:HB3	1:A:1163:ARG:NH1	2.08	0.67
1:B:2102:HIS:ND1	1:B:2103:ARG:HG2	2.09	0.67
1:D:4039:MET:HG3	1:D:4048:ILE:CD1	2.24	0.67
1:C:3155:GLY:HA3	1:C:3161:ASN:HB2	1.76	0.67
1:D:4193:ASN:HD21	1:D:4249:GLY:H	1.43	0.67
1:B:2039:MET:HG3	1:B:2048:ILE:CD1	2.24	0.67
1:F:6039:MET:HG3	1:F:6048:ILE:CD1	2.20	0.67
1:A:1011:SER:N	1:C:3007:GLN:HE22	1.87	0.66
1:C:3152:VAL:HG12	1:C:3154:LEU:HD13	1.77	0.66
1:D:4155:GLY:HA3	1:D:4161:ASN:HB2	1.78	0.66
1:F:6155:GLY:HA3	1:F:6161:ASN:HB2	1.78	0.66
1:D:4230:HIS:HD2	1:F:6230:HIS:HD2	1.42	0.66
1:E:5155:GLY:HA3	1:E:5161:ASN:HB2	1.77	0.66
1:A:1211:ASN:HD22	1:A:1256:THR:HG21	1.61	0.65
1:F:6102:HIS:ND1	1:F:6103:ARG:HG2	2.11	0.65
1:F:6101:GLY:O	1:F:6104:ASP:HB2	1.97	0.65
1:F:6100:ILE:HD12	1:F:6100:ILE:H	1.61	0.65
1:D:4100:ILE:HD12	1:D:4100:ILE:H	1.62	0.64
1:D:4102:HIS:ND1	1:D:4103:ARG:HG2	2.13	0.64
1:D:4162:ARG:HG2	1:D:4162:ARG:HH11	1.62	0.64
1:F:6152:VAL:HG12	1:F:6154:LEU:HD13	1.78	0.64
1:A:1100:ILE:HD12	1:A:1100:ILE:H	1.63	0.64
1:A:1102:HIS:ND1	1:A:1103:ARG:HG2	2.13	0.64
1:A:1155:GLY:HA3	1:A:1161:ASN:HB2	1.79	0.64
1:E:5100:ILE:HD12	1:E:5100:ILE:H	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3182:GLY:HA3	1:C:3259:TRP:CZ2	2.33	0.64
1:F:6047:ILE:HD11	1:F:6262:VAL:HG11	1.79	0.64
1:A:1039:MET:HG3	1:A:1048:ILE:CD1	2.23	0.63
1:E:5149:VAL:HG11	1:E:5166:ASN:HB3	1.80	0.63
1:A:1157:ASN:N	1:A:1157:ASN:ND2	2.44	0.63
1:E:5152:VAL:HG12	1:E:5154:LEU:HD13	1.79	0.63
1:E:5168:TYR:O	1:E:5173:VAL:HG11	1.98	0.63
1:A:1152:VAL:HG12	1:A:1154:LEU:HD13	1.79	0.63
1:F:6057:LYS:HG2	1:F:6058:THR:H	1.63	0.63
1:B:2155:GLY:HA3	1:B:2161:ASN:HB2	1.81	0.63
1:D:4152:VAL:HG12	1:D:4154:LEU:HD13	1.81	0.63
1:F:6168:TYR:O	1:F:6173:VAL:HG11	1.99	0.63
1:E:5193:ASN:HD21	1:E:5249:GLY:N	1.96	0.62
1:E:5047:ILE:HD11	1:E:5262:VAL:CG1	2.22	0.62
1:E:5204:MET:HE1	1:E:5240:ILE:HG23	1.82	0.62
1:B:2101:GLY:O	1:B:2104:ASP:HB2	1.99	0.62
1:B:2182:GLY:HA3	1:B:2259:TRP:CZ2	2.35	0.62
1:B:2192:TRP:CZ3	1:B:2250:VAL:HG22	2.35	0.62
1:C:3101:GLY:O	1:C:3104:ASP:HB2	1.99	0.62
1:E:5091:ILE:HD12	1:E:5117:PHE:CE1	2.35	0.62
1:B:2157:ASN:N	1:B:2157:ASN:ND2	2.43	0.62
1:B:2193:ASN:HD21	1:B:2249:GLY:H	1.48	0.62
1:F:6162:ARG:HG2	1:F:6162:ARG:HH11	1.65	0.62
1:A:1136:HIS:CD2	1:C:3177:CYS:HB3	2.34	0.62
1:A:1193:ASN:O	1:A:1194:THR:HG23	2.00	0.61
1:C:3039:MET:HG3	1:C:3048:ILE:CD1	2.28	0.61
1:A:1192:TRP:CE2	1:A:1250:VAL:HG13	2.36	0.61
1:B:2057:LYS:HG2	1:B:2058:THR:H	1.65	0.61
1:D:4168:TYR:O	1:D:4173:VAL:HG11	2.01	0.61
1:B:2152:VAL:HG12	1:B:2154:LEU:HD13	1.81	0.61
1:E:5182:GLY:HA3	1:E:5259:TRP:CZ2	2.35	0.61
1:B:2157:ASN:ND2	1:B:2157:ASN:H	1.97	0.61
1:C:3162:ARG:HG2	1:C:3162:ARG:HH11	1.64	0.61
1:F:6157:ASN:N	1:F:6157:ASN:ND2	2.45	0.61
1:A:1162:ARG:HG2	1:A:1162:ARG:HH11	1.66	0.60
1:A:1193:ASN:HD21	1:A:1249:GLY:N	1.98	0.60
1:C:3183:LEU:C	1:C:3183:LEU:HD23	2.26	0.60
1:E:5162:ARG:HG2	1:E:5162:ARG:HH11	1.65	0.60
1:C:3157:ASN:N	1:C:3157:ASN:ND2	2.45	0.60
1:C:3193:ASN:O	1:C:3194:THR:HG23	2.01	0.60
1:C:3100:ILE:HD12	1:C:3100:ILE:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3149:VAL:HG11	1:C:3166:ASN:HB3	1.84	0.60
1:D:4183:LEU:C	1:D:4183:LEU:HD23	2.27	0.60
1:F:6149:VAL:HG11	1:F:6166:ASN:HB3	1.84	0.60
1:E:5057:LYS:HG2	1:E:5058:THR:H	1.66	0.60
1:D:4182:GLY:HA3	1:D:4259:TRP:CZ2	2.36	0.60
1:C:3057:LYS:HG2	1:C:3058:THR:H	1.66	0.60
1:D:4193:ASN:HD21	1:D:4249:GLY:N	1.99	0.60
1:A:1192:TRP:CH2	1:A:1250:VAL:HG22	2.37	0.60
1:B:2193:ASN:O	1:B:2194:THR:HG23	2.02	0.60
1:B:2100:ILE:HD12	1:B:2100:ILE:H	1.66	0.59
1:B:2183:LEU:C	1:B:2183:LEU:HD23	2.27	0.59
1:F:6211:ASN:HD22	1:F:6256:THR:HG21	1.67	0.59
1:A:1149:VAL:HG11	1:A:1166:ASN:HB3	1.84	0.59
1:F:6183:LEU:C	1:F:6183:LEU:HD23	2.27	0.59
1:A:1057:LYS:HG2	1:A:1058:THR:H	1.66	0.59
1:B:2162:ARG:HG2	1:B:2162:ARG:HH11	1.66	0.59
1:D:4091:ILE:HD12	1:D:4117:PHE:CE1	2.37	0.59
1:D:4211:ASN:HD22	1:D:4256:THR:HG21	1.68	0.59
1:C:3157:ASN:ND2	1:C:3157:ASN:H	2.00	0.59
1:D:4057:LYS:HG2	1:D:4058:THR:H	1.68	0.59
1:E:5157:ASN:N	1:E:5157:ASN:ND2	2.47	0.59
1:D:4149:VAL:HG11	1:D:4166:ASN:HB3	1.84	0.59
1:E:5085:ILE:HG13	1:E:5210:PHE:CE2	2.36	0.59
1:C:3204:MET:HE1	1:C:3240:ILE:HG23	1.83	0.58
1:D:4230:HIS:HD2	1:F:6230:HIS:CD2	2.21	0.58
1:F:6193:ASN:O	1:F:6194:THR:HG23	2.03	0.58
1:C:3168:TYR:O	1:C:3173:VAL:HG11	2.03	0.58
1:A:1209:TYR:OH	1:A:1220:HIS:HD2	1.85	0.58
1:D:4157:ASN:N	1:D:4157:ASN:ND2	2.51	0.58
1:C:3091:ILE:HD12	1:C:3117:PHE:CE1	2.39	0.58
1:D:4193:ASN:O	1:D:4194:THR:HG23	2.04	0.58
1:A:1157:ASN:ND2	1:A:1157:ASN:H	1.99	0.58
1:A:1183:LEU:C	1:A:1183:LEU:HD23	2.29	0.58
1:A:1136:HIS:H	1:C:3136:HIS:CD2	2.15	0.57
1:E:5193:ASN:ND2	1:E:5249:GLY:H	2.00	0.57
1:A:1212:MET:HE1	1:A:1218:VAL:HG23	1.85	0.57
1:F:6204:MET:SD	1:F:6204:MET:C	2.87	0.57
1:A:1101:GLY:O	1:A:1104:ASP:HB2	2.04	0.57
1:B:2149:VAL:HG11	1:B:2166:ASN:HB3	1.85	0.57
1:F:6091:ILE:HD12	1:F:6117:PHE:CE1	2.39	0.57
1:F:6157:ASN:ND2	1:F:6157:ASN:H	2.01	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4228:THR:OG1	1:F:6230:HIS:HE1	1.87	0.57
1:D:4091:ILE:HG22	1:D:4100:ILE:HG13	1.87	0.57
1:A:1177:CYS:HB3	1:C:3136:HIS:CD2	2.39	0.57
1:E:5193:ASN:O	1:E:5194:THR:HG23	2.04	0.57
1:F:6086:GLY:O	1:F:6102:HIS:HD2	1.86	0.57
1:B:2193:ASN:HD21	1:B:2249:GLY:N	2.03	0.57
1:D:4230:HIS:CD2	1:F:6230:HIS:HD2	2.23	0.57
1:A:1091:ILE:HD12	1:A:1117:PHE:CE1	2.39	0.57
1:C:3091:ILE:HG22	1:C:3100:ILE:HG13	1.87	0.56
1:D:4193:ASN:ND2	1:D:4249:GLY:H	2.03	0.56
1:B:2091:ILE:HD12	1:B:2117:PHE:CE1	2.41	0.56
1:C:3091:ILE:CD1	1:C:3106:LEU:HD23	2.33	0.56
1:A:1192:TRP:CH2	1:A:1250:VAL:CG2	2.89	0.56
1:A:1193:ASN:ND2	1:A:1249:GLY:H	2.04	0.56
1:E:5157:ASN:ND2	1:E:5157:ASN:H	2.04	0.56
1:F:6182:GLY:HA3	1:F:6259:TRP:CZ2	2.40	0.56
1:B:2168:TYR:O	1:B:2173:VAL:HG11	2.06	0.56
1:E:5183:LEU:C	1:E:5183:LEU:HD23	2.31	0.56
1:F:6193:ASN:HD21	1:F:6249:GLY:H	1.53	0.55
1:D:4193:ASN:HD22	1:D:4193:ASN:H	1.55	0.55
1:E:5192:TRP:CE2	1:E:5250:VAL:HG13	2.41	0.55
1:E:5091:ILE:HG22	1:E:5100:ILE:HG13	1.88	0.55
1:E:5192:TRP:CH2	1:E:5250:VAL:CG2	2.89	0.55
1:A:1205:GLU:OE2	1:A:1247:HIS:NE2	2.39	0.55
1:A:1091:ILE:HG22	1:A:1100:ILE:HG13	1.89	0.55
1:F:6091:ILE:HD13	1:F:6106:LEU:CD2	2.34	0.55
1:A:1086:GLY:O	1:A:1102:HIS:HD2	1.89	0.55
1:C:3193:ASN:HD22	1:C:3193:ASN:H	1.55	0.55
1:D:4086:GLY:O	1:D:4102:HIS:HD2	1.90	0.54
1:F:6170:VAL:H	1:F:6173:VAL:CG1	2.21	0.54
1:E:5192:TRP:CH2	1:E:5250:VAL:HG22	2.43	0.54
1:B:2157:ASN:HD22	1:B:2157:ASN:H	1.53	0.54
1:F:6091:ILE:CD1	1:F:6106:LEU:HD23	2.34	0.54
1:D:4230:HIS:CE1	1:F:6228:THR:OG1	2.57	0.54
1:B:2086:GLY:O	1:B:2102:HIS:HD2	1.91	0.54
1:E:5186:LEU:HD12	1:E:5255:TYR:CE1	2.43	0.53
1:E:5216:ALA:O	1:E:5217:CYS:HB3	2.09	0.53
1:B:2193:ASN:HD22	1:B:2193:ASN:H	1.55	0.53
1:D:4019:THR:HB	1:F:6227:GLU:OE2	2.07	0.53
1:F:6091:ILE:HG22	1:F:6100:ILE:HG13	1.90	0.53
1:F:6193:ASN:HD22	1:F:6193:ASN:H	1.55	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2163:ARG:HB3	1:B:2186:LEU:CD2	2.26	0.53
1:D:4048:ILE:HD12	1:D:4049:VAL:N	2.24	0.53
1:A:1046:ARG:HH11	1:A:1046:ARG:HG3	1.74	0.53
1:C:3170:VAL:H	1:C:3173:VAL:CG1	2.22	0.53
1:D:4120:ILE:O	1:D:4121:ASP:HB2	2.08	0.53
1:B:2167:LYS:HE3	1:B:2268:PHE:HD2	1.74	0.53
1:C:3091:ILE:HD13	1:C:3106:LEU:CD2	2.33	0.53
1:D:4170:VAL:H	1:D:4173:VAL:CG1	2.21	0.53
1:E:5203:ARG:HG3	1:E:5203:ARG:O	2.09	0.53
1:B:2046:ARG:HH11	1:B:2046:ARG:HG3	1.74	0.53
1:B:2193:ASN:ND2	1:B:2249:GLY:H	2.06	0.53
1:E:5089:GLY:O	1:E:5100:ILE:HD12	2.09	0.52
1:C:3120:ILE:O	1:C:3121:ASP:HB2	2.09	0.52
1:E:5046:ARG:HH11	1:E:5046:ARG:HG3	1.74	0.52
1:F:6046:ARG:HH11	1:F:6046:ARG:HG3	1.74	0.52
1:A:1193:ASN:HD22	1:A:1193:ASN:H	1.57	0.52
1:C:3086:GLY:O	1:C:3102:HIS:HD2	1.92	0.52
1:E:5091:ILE:CD1	1:E:5106:LEU:HD23	2.35	0.52
1:C:3046:ARG:HH11	1:C:3046:ARG:HG3	1.75	0.52
1:D:4203:ARG:NH1	1:D:4205:GLU:OE1	2.42	0.52
1:F:6120:ILE:O	1:F:6121:ASP:HB2	2.08	0.52
1:A:1163:ARG:HB3	1:A:1186:LEU:CD2	2.25	0.52
1:D:4046:ARG:HH11	1:D:4046:ARG:HG3	1.74	0.52
1:E:5104:ASP:OD2	1:E:5145:THR:HG22	2.10	0.52
1:B:2091:ILE:HG22	1:B:2100:ILE:HG13	1.90	0.52
1:F:6209:TYR:OH	1:F:6220:HIS:HD2	1.92	0.52
1:B:2089:GLY:O	1:B:2100:ILE:HD12	2.09	0.52
1:E:5086:GLY:O	1:E:5102:HIS:HD2	1.92	0.52
1:E:5170:VAL:H	1:E:5173:VAL:CG1	2.22	0.52
1:A:1168:TYR:O	1:A:1173:VAL:HG11	2.09	0.51
1:A:1211:ASN:HD22	1:A:1256:THR:CG2	2.22	0.51
1:D:4227:GLU:HA	1:F:6019:THR:OG1	2.10	0.51
1:A:1165:ILE:HG22	1:A:1184:THR:OG1	2.10	0.51
1:E:5120:ILE:O	1:E:5121:ASP:HB2	2.09	0.51
1:B:2048:ILE:HD12	1:B:2049:VAL:N	2.25	0.51
1:B:2120:ILE:O	1:B:2121:ASP:HB2	2.09	0.51
1:C:3192:TRP:CZ3	1:C:3250:VAL:HG22	2.45	0.51
1:D:4047:ILE:HD11	1:D:4262:VAL:CG1	2.30	0.51
1:F:6193:ASN:HD21	1:F:6249:GLY:N	2.09	0.51
1:E:5193:ASN:HD22	1:E:5193:ASN:H	1.59	0.51
1:A:1157:ASN:HD22	1:A:1157:ASN:H	1.55	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2170:VAL:H	1:B:2173:VAL:CG1	2.23	0.51
1:C:3090:THR:HG22	1:C:3118:ALA:HB3	1.93	0.51
1:F:6041:TYR:OH	1:F:6046:ARG:HG2	2.10	0.51
1:F:6154:LEU:O	1:F:6162:ARG:HA	2.10	0.51
1:D:4091:ILE:HD13	1:D:4106:LEU:CD2	2.37	0.51
1:F:6193:ASN:ND2	1:F:6249:GLY:H	2.09	0.51
1:D:4137:THR:HG21	1:E:5162:ARG:HH12	1.76	0.51
1:F:6110:LYS:HB3	1:F:6138:THR:HG22	1.93	0.51
1:B:2170:VAL:HG23	1:B:2173:VAL:HG12	1.93	0.51
1:B:2193:ASN:HD22	1:B:2193:ASN:N	2.09	0.51
1:C:3041:TYR:OH	1:C:3046:ARG:HG2	2.10	0.51
1:A:1170:VAL:H	1:A:1173:VAL:CG1	2.24	0.51
1:B:2212:MET:HE1	1:B:2218:VAL:HG23	1.93	0.51
1:C:3211:ASN:HD22	1:C:3256:THR:HG21	1.75	0.50
1:F:6211:ASN:HD22	1:F:6256:THR:CG2	2.24	0.50
1:A:1120:ILE:O	1:A:1121:ASP:HB2	2.11	0.50
1:A:1186:LEU:HD12	1:A:1255:TYR:CE1	2.47	0.50
1:A:1048:ILE:HD12	1:A:1049:VAL:N	2.26	0.50
1:D:4157:ASN:ND2	1:D:4157:ASN:H	2.09	0.50
1:D:4186:LEU:HD12	1:D:4255:TYR:CE1	2.47	0.50
1:D:4192:TRP:CH2	1:D:4250:VAL:HG22	2.47	0.50
1:A:1045:ASP:OD1	1:C:3046:ARG:NH1	2.45	0.50
1:D:4162:ARG:HH11	1:D:4162:ARG:CG	2.24	0.50
1:D:4207:TYR:O	1:D:4238:ALA:HA	2.11	0.50
1:E:5054:PRO:HG2	1:E:5119:SER:OG	2.12	0.50
1:F:6048:ILE:HD12	1:F:6049:VAL:N	2.27	0.50
1:F:6165:ILE:HG22	1:F:6184:THR:OG1	2.12	0.50
1:F:6193:ASN:HD22	1:F:6193:ASN:N	2.08	0.50
1:C:3052:ILE:HD13	1:C:3117:PHE:CD2	2.47	0.50
1:A:1047:ILE:CD1	1:A:1133:ALA:HB2	2.42	0.50
1:D:4154:LEU:O	1:D:4162:ARG:HA	2.12	0.50
1:C:3110:LYS:CG	1:C:3138:THR:HG22	2.42	0.50
1:D:4110:LYS:CG	1:D:4138:THR:HG22	2.42	0.50
1:F:6089:GLY:O	1:F:6100:ILE:HD12	2.12	0.50
1:C:3162:ARG:HH11	1:C:3162:ARG:CG	2.25	0.49
1:D:4192:TRP:CH2	1:D:4250:VAL:CG2	2.95	0.49
1:B:2154:LEU:O	1:B:2162:ARG:HA	2.12	0.49
1:D:4089:GLY:O	1:D:4100:ILE:HD12	2.12	0.49
1:E:5162:ARG:HH11	1:E:5162:ARG:CG	2.25	0.49
1:A:1091:ILE:HD13	1:A:1106:LEU:CD2	2.38	0.49
1:A:1110:LYS:CG	1:A:1138:THR:HG22	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5110:LYS:HB3	1:E:5138:THR:HG22	1.93	0.49
1:E:5154:LEU:O	1:E:5162:ARG:HA	2.12	0.49
1:B:2085:ILE:HG13	1:B:2210:PHE:CE2	2.47	0.49
1:C:3193:ASN:HD21	1:C:3249:GLY:H	1.60	0.49
1:D:4227:GLU:OE1	1:D:4229:ARG:NH2	2.45	0.49
1:C:3048:ILE:HD12	1:C:3049:VAL:N	2.28	0.49
1:C:3227:GLU:OE1	1:C:3229:ARG:NH2	2.45	0.49
1:B:2203:ARG:O	1:B:2203:ARG:HG3	2.13	0.49
1:E:5110:LYS:CG	1:E:5138:THR:HG22	2.43	0.49
1:F:6110:LYS:O	1:F:6138:THR:HB	2.13	0.49
1:A:1136:HIS:HD2	1:C:3136:HIS:H	1.59	0.48
1:A:1154:LEU:O	1:A:1162:ARG:HA	2.13	0.48
1:B:2091:ILE:CD1	1:B:2106:LEU:HD23	2.38	0.48
1:E:5131:ASN:ND2	1:E:5260:GLY:HA3	2.28	0.48
1:F:6204:MET:O	1:F:6205:GLU:HG3	2.13	0.48
1:C:3089:GLY:O	1:C:3100:ILE:HD12	2.13	0.48
1:D:4054:PRO:HG2	1:D:4119:SER:OG	2.12	0.48
1:A:1193:ASN:HD22	1:A:1193:ASN:N	2.10	0.48
1:C:3193:ASN:HD22	1:C:3193:ASN:N	2.09	0.48
1:E:5052:ILE:HD13	1:E:5117:PHE:CD2	2.49	0.48
1:E:5165:ILE:HG22	1:E:5184:THR:OG1	2.13	0.48
1:F:6110:LYS:CG	1:F:6138:THR:HG22	2.43	0.48
1:B:2110:LYS:CG	1:B:2138:THR:HG22	2.44	0.48
1:C:3054:PRO:HG2	1:C:3119:SER:OG	2.13	0.48
1:F:6227:GLU:OE1	1:F:6229:ARG:NH2	2.46	0.48
1:A:1136:HIS:N	1:C:3136:HIS:HD2	2.02	0.48
1:C:3154:LEU:O	1:C:3162:ARG:HA	2.13	0.48
1:D:4019:THR:OG1	1:F:6227:GLU:HA	2.14	0.48
1:E:5170:VAL:HG23	1:E:5173:VAL:HG12	1.96	0.48
1:A:1215:ASP:OD2	1:A:1216:ALA:N	2.47	0.48
1:C:3091:ILE:CG2	1:C:3106:LEU:HD22	2.44	0.48
1:D:4027:LEU:HD22	1:D:4028:VAL:N	2.29	0.48
1:D:4204:MET:SD	1:D:4204:MET:C	2.97	0.48
1:E:5048:ILE:HD12	1:E:5049:VAL:N	2.29	0.48
1:E:5227:GLU:OE1	1:E:5229:ARG:NH2	2.46	0.48
1:A:1015:LYS:HE3	1:A:1227:GLU:CD	2.38	0.48
1:D:4047:ILE:CD1	1:D:4133:ALA:HB2	2.43	0.48
1:F:6210:PHE:CE1	1:F:6258:ILE:HG12	2.49	0.48
1:A:1170:VAL:HG23	1:A:1172:ASP:OD2	2.14	0.48
1:B:2192:TRP:CH2	1:B:2250:VAL:HG22	2.48	0.48
1:B:2207:TYR:O	1:B:2238:ALA:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2162:ARG:HH11	1:B:2162:ARG:CG	2.27	0.48
1:A:1052:ILE:HD13	1:A:1117:PHE:CD2	2.49	0.47
1:A:1182:GLY:HA3	1:A:1259:TRP:CZ2	2.48	0.47
1:B:2054:PRO:HG2	1:B:2119:SER:OG	2.14	0.47
1:A:1085:ILE:HG13	1:A:1210:PHE:CE2	2.49	0.47
1:A:1091:ILE:CD1	1:A:1106:LEU:HD23	2.37	0.47
1:B:2182:GLY:HA3	1:B:2259:TRP:CE2	2.49	0.47
1:F:6091:ILE:CG2	1:F:6106:LEU:HD22	2.45	0.47
1:B:2104:ASP:OD2	1:B:2145:THR:HG22	2.14	0.47
1:D:4110:LYS:HB3	1:D:4138:THR:HG22	1.97	0.47
1:E:5192:TRP:CH2	1:E:5250:VAL:HG21	2.50	0.47
1:F:6057:LYS:HG2	1:F:6058:THR:N	2.28	0.47
1:F:6104:ASP:OD2	1:F:6145:THR:HG22	2.13	0.47
1:F:6203:ARG:O	1:F:6203:ARG:HG3	2.13	0.47
1:A:1031:VAL:HG21	1:A:1208:PHE:HE2	1.79	0.47
1:B:2165:ILE:HG22	1:B:2184:THR:OG1	2.15	0.47
1:C:3165:ILE:HG22	1:C:3184:THR:OG1	2.14	0.47
1:D:4192:TRP:CE2	1:D:4250:VAL:HG13	2.49	0.47
1:E:5110:LYS:O	1:E:5138:THR:HB	2.15	0.47
1:A:1031:VAL:HG21	1:A:1208:PHE:CE2	2.50	0.47
1:A:1089:GLY:O	1:A:1100:ILE:HD12	2.15	0.47
1:B:2057:LYS:HG2	1:B:2058:THR:N	2.30	0.47
1:C:3057:LYS:HG2	1:C:3058:THR:N	2.30	0.47
1:C:3170:VAL:HG23	1:C:3172:ASP:OD2	2.15	0.47
1:D:4104:ASP:OD2	1:D:4145:THR:HG22	2.15	0.47
1:D:4110:LYS:O	1:D:4138:THR:HB	2.15	0.47
1:E:5041:TYR:OH	1:E:5046:ARG:HG2	2.15	0.47
1:E:5182:GLY:HA3	1:E:5259:TRP:CE2	2.49	0.47
1:F:6052:ILE:HD13	1:F:6117:PHE:CD2	2.50	0.47
1:F:6151:PRO:HB3	1:F:6166:ASN:ND2	2.29	0.47
1:F:6162:ARG:HH11	1:F:6162:ARG:CG	2.26	0.47
1:B:2227:GLU:OE1	1:B:2229:ARG:NH2	2.47	0.47
1:D:4131:ASN:ND2	1:D:4260:GLY:HA3	2.30	0.47
1:F:6170:VAL:HG23	1:F:6172:ASP:OD2	2.15	0.47
1:A:1140:PRO:HD3	1:D:4158:LEU:CD1	2.45	0.47
1:D:4204:MET:HE2	1:D:4204:MET:HB2	1.72	0.47
1:E:5211:ASN:HD22	1:E:5256:THR:CG2	2.25	0.47
1:B:2052:ILE:HD13	1:B:2117:PHE:CD2	2.50	0.47
1:D:4204:MET:HE1	1:D:4240:ILE:CG2	2.45	0.47
1:E:5047:ILE:CD1	1:E:5262:VAL:HG11	2.27	0.46
1:B:2031:VAL:HG21	1:B:2208:PHE:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4038:THR:HB	1:D:4051:GLY:H	1.81	0.46
1:D:4090:THR:HG22	1:D:4118:ALA:HB3	1.97	0.46
1:D:4170:VAL:HG23	1:D:4173:VAL:HG12	1.98	0.46
1:D:4182:GLY:HA3	1:D:4259:TRP:CE2	2.51	0.46
1:C:3153:THR:O	1:C:3154:LEU:HD12	2.15	0.46
1:D:4193:ASN:HD22	1:D:4193:ASN:N	2.09	0.46
1:D:4003:LEU:HD11	1:D:4039:MET:HG2	1.98	0.46
1:D:4057:LYS:HG2	1:D:4058:THR:N	2.31	0.46
1:D:4167:LYS:HE3	1:D:4268:PHE:HD2	1.80	0.46
1:C:3085:ILE:HG13	1:C:3210:PHE:CE2	2.51	0.46
1:D:4161:ASN:N	1:D:4161:ASN:HD22	2.12	0.46
1:E:5090:THR:HG22	1:E:5118:ALA:HB3	1.98	0.46
1:F:6057:LYS:CG	1:F:6058:THR:H	2.28	0.46
1:B:2091:ILE:HD13	1:B:2106:LEU:CD2	2.38	0.46
1:C:3161:ASN:O	1:C:3162:ARG:C	2.59	0.46
1:E:5027:LEU:HD22	1:E:5028:VAL:N	2.31	0.46
1:F:6187:ALA:O	1:F:6188:PRO:C	2.59	0.46
1:E:5057:LYS:HG2	1:E:5058:THR:N	2.29	0.46
1:F:6192:TRP:CZ3	1:F:6250:VAL:HG22	2.51	0.46
1:A:1057:LYS:HG2	1:A:1058:THR:N	2.30	0.46
1:A:1090:THR:HG22	1:A:1118:ALA:HB3	1.98	0.46
1:B:2193:ASN:H	1:B:2193:ASN:ND2	2.14	0.46
1:E:5193:ASN:HD22	1:E:5193:ASN:N	2.12	0.46
1:C:3102:HIS:CE1	1:C:3103:ARG:HD3	2.51	0.46
1:E:5102:HIS:CE1	1:E:5103:ARG:HD3	2.51	0.46
1:E:5187:ALA:O	1:E:5188:PRO:C	2.57	0.46
1:C:3104:ASP:OD2	1:C:3145:THR:HG22	2.15	0.46
1:C:3193:ASN:H	1:C:3193:ASN:ND2	2.14	0.46
1:D:4161:ASN:O	1:D:4162:ARG:C	2.58	0.46
1:E:5163:ARG:HB3	1:E:5186:LEU:CD2	2.25	0.46
1:A:1110:LYS:HB3	1:A:1138:THR:HG22	1.98	0.45
1:A:1227:GLU:OE1	1:A:1229:ARG:NH2	2.49	0.45
1:D:4091:ILE:CG2	1:D:4106:LEU:HD22	2.46	0.45
1:F:6054:PRO:HG2	1:F:6119:SER:OG	2.16	0.45
1:A:1054:PRO:HG2	1:A:1119:SER:OG	2.15	0.45
1:B:2110:LYS:O	1:B:2138:THR:HB	2.15	0.45
1:C:3152:VAL:HB	1:C:3165:ILE:HG13	1.98	0.45
1:E:5091:ILE:HD13	1:E:5106:LEU:CD2	2.38	0.45
1:A:1187:ALA:O	1:A:1188:PRO:C	2.58	0.45
1:E:5091:ILE:CG2	1:E:5106:LEU:HD22	2.46	0.45
1:F:6163:ARG:HB3	1:F:6186:LEU:CD2	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6193:ASN:H	1:F:6193:ASN:ND2	2.14	0.45
1:A:1161:ASN:N	1:A:1161:ASN:HD22	2.14	0.45
1:C:3091:ILE:HG22	1:C:3100:ILE:CG1	2.46	0.45
1:C:3110:LYS:HB3	1:C:3138:THR:HG22	1.98	0.45
1:D:4049:VAL:HG21	1:D:4206:VAL:HG11	1.98	0.45
1:D:4091:ILE:CD1	1:D:4106:LEU:HD23	2.37	0.45
1:A:1152:VAL:HB	1:A:1165:ILE:HG13	1.99	0.45
1:B:2047:ILE:CD1	1:B:2133:ALA:HB2	2.46	0.45
1:A:1162:ARG:HH11	1:A:1162:ARG:CG	2.28	0.45
1:D:4228:THR:OG1	1:F:6230:HIS:CE1	2.68	0.45
1:F:6090:THR:HG22	1:F:6118:ALA:HB3	1.99	0.45
1:F:6047:ILE:CD1	1:F:6133:ALA:HB2	2.46	0.45
1:B:2091:ILE:CG2	1:B:2106:LEU:HD22	2.47	0.45
1:B:2187:ALA:O	1:B:2188:PRO:C	2.60	0.45
1:F:6032:PHE:CE1	1:F:6127:LYS:HB3	2.51	0.45
1:D:4165:ILE:HG22	1:D:4184:THR:OG1	2.17	0.45
1:B:2057:LYS:CG	1:B:2058:THR:H	2.30	0.45
1:C:3193:ASN:HD21	1:C:3249:GLY:N	2.15	0.45
1:A:1091:ILE:CG2	1:A:1106:LEU:HD22	2.48	0.44
1:C:3151:PRO:HB3	1:C:3166:ASN:ND2	2.31	0.44
1:C:3187:ALA:O	1:C:3188:PRO:C	2.60	0.44
1:D:4009:ILE:HD11	1:D:4026:PHE:HZ	1.82	0.44
1:A:1041:TYR:OH	1:A:1046:ARG:HG2	2.16	0.44
1:B:2192:TRP:CH2	1:B:2250:VAL:CG2	3.00	0.44
1:D:4187:ALA:O	1:D:4188:PRO:C	2.59	0.44
1:A:1003:LEU:HD11	1:A:1039:MET:HG2	1.98	0.44
1:A:1057:LYS:CG	1:A:1058:THR:H	2.29	0.44
1:A:1178:GLN:HG3	1:C:3136:HIS:CE1	2.52	0.44
1:B:2148:GLU:H	1:B:2148:GLU:HG2	1.53	0.44
1:C:3163:ARG:HB3	1:C:3186:LEU:CD2	2.27	0.44
1:D:4220:HIS:O	1:D:4230:HIS:HA	2.17	0.44
1:E:5091:ILE:HG22	1:E:5100:ILE:CG1	2.48	0.44
1:E:5153:THR:O	1:E:5154:LEU:HD12	2.17	0.44
1:E:5167:LYS:HE3	1:E:5268:PHE:HD2	1.82	0.44
1:E:5265:ASN:ND2	1:E:5267:VAL:HB	2.32	0.44
1:C:3110:LYS:O	1:C:3138:THR:HB	2.17	0.44
1:D:4085:ILE:HG13	1:D:4210:PHE:CE2	2.52	0.44
1:D:4163:ARG:HB3	1:D:4186:LEU:CD2	2.26	0.44
1:A:1193:ASN:ND2	1:A:1193:ASN:H	2.15	0.44
1:E:5003:LEU:HD11	1:E:5039:MET:HG2	2.00	0.44
1:F:6091:ILE:HG21	1:F:6106:LEU:HD22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:ILE:HG22	1:A:1100:ILE:CG1	2.46	0.44
1:C:3047:ILE:CD1	1:C:3133:ALA:HB2	2.48	0.44
1:E:5161:ASN:HD22	1:E:5161:ASN:N	2.14	0.44
1:F:6152:VAL:HB	1:F:6165:ILE:HG13	2.00	0.44
1:D:4161:ASN:N	1:D:4161:ASN:ND2	2.65	0.44
1:B:2003:LEU:HD11	1:B:2039:MET:HG2	2.00	0.44
1:B:2038:THR:HB	1:B:2051:GLY:H	1.83	0.44
1:E:5212:MET:C	1:E:5213:ASP:O	2.60	0.44
1:B:2120:ILE:O	1:B:2120:ILE:HG13	2.18	0.44
1:C:3003:LEU:HD11	1:C:3039:MET:HG2	2.00	0.44
1:D:4032:PHE:CE1	1:D:4127:LYS:HB3	2.53	0.44
1:D:4052:ILE:HD13	1:D:4117:PHE:CD2	2.53	0.44
1:D:4161:ASN:HB2	1:D:4162:ARG:H	1.59	0.44
1:F:6161:ASN:N	1:F:6161:ASN:HD22	2.15	0.44
1:A:1037:TYR:CD1	1:A:1037:TYR:C	2.96	0.43
1:A:1170:VAL:HG23	1:A:1173:VAL:HG12	2.00	0.43
1:B:2032:PHE:CE1	1:B:2127:LYS:HB3	2.53	0.43
1:C:3032:PHE:CE1	1:C:3127:LYS:HB3	2.53	0.43
1:C:3161:ASN:HB2	1:C:3162:ARG:H	1.62	0.43
1:E:5057:LYS:CG	1:E:5058:THR:H	2.30	0.43
1:E:5220:HIS:O	1:E:5230:HIS:HA	2.18	0.43
1:A:1110:LYS:O	1:A:1138:THR:HB	2.18	0.43
1:B:2041:TYR:OH	1:B:2046:ARG:HG2	2.17	0.43
1:D:4162:ARG:CG	1:D:4162:ARG:NH1	2.80	0.43
1:E:5032:PHE:CE1	1:E:5127:LYS:HB3	2.54	0.43
1:D:4193:ASN:ND2	1:D:4193:ASN:H	2.14	0.43
1:F:6186:LEU:HD12	1:F:6255:TYR:CE1	2.53	0.43
1:A:1010:HIS:HB2	1:C:3009:ILE:HG22	2.00	0.43
1:C:3091:ILE:HD12	1:C:3117:PHE:HE1	1.82	0.43
1:D:4152:VAL:HB	1:D:4165:ILE:HG13	1.99	0.43
1:F:6091:ILE:HD12	1:F:6117:PHE:HE1	1.83	0.43
1:B:2161:ASN:N	1:B:2161:ASN:HD22	2.16	0.43
1:B:2186:LEU:HD12	1:B:2255:TYR:CE1	2.53	0.43
1:D:4037:TYR:CD1	1:D:4037:TYR:C	2.96	0.43
1:D:4041:TYR:OH	1:D:4046:ARG:HG2	2.19	0.43
1:F:6210:PHE:HE1	1:F:6258:ILE:HG12	1.82	0.43
1:B:2051:GLY:C	1:B:2052:ILE:HG13	2.44	0.43
1:B:2110:LYS:HB3	1:B:2138:THR:HG22	2.01	0.43
1:B:2152:VAL:HB	1:B:2165:ILE:HG13	2.00	0.43
1:C:3193:ASN:ND2	1:C:3249:GLY:H	2.16	0.43
1:C:3210:PHE:CE1	1:C:3258:ILE:HG12	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5161:ASN:HB2	1:E:5162:ARG:H	1.59	0.43
1:E:5193:ASN:ND2	1:E:5193:ASN:H	2.17	0.43
1:A:1032:PHE:CE1	1:A:1127:LYS:HB3	2.53	0.43
1:C:3027:LEU:HD22	1:C:3028:VAL:N	2.34	0.43
1:D:4153:THR:O	1:D:4154:LEU:HD12	2.19	0.43
1:F:6182:GLY:HA3	1:F:6259:TRP:CE2	2.54	0.43
1:E:5047:ILE:CD1	1:E:5133:ALA:HB2	2.49	0.43
1:E:5091:ILE:HD12	1:E:5117:PHE:HE1	1.78	0.43
1:F:6027:LEU:HD22	1:F:6028:VAL:N	2.33	0.43
1:F:6161:ASN:N	1:F:6161:ASN:ND2	2.67	0.43
1:B:2131:ASN:HB2	1:B:2181:MET:SD	2.59	0.43
1:F:6085:ILE:HG13	1:F:6210:PHE:CE2	2.54	0.43
1:A:1027:LEU:HD22	1:A:1028:VAL:N	2.34	0.43
1:C:3091:ILE:HG21	1:C:3106:LEU:HD22	2.00	0.43
1:E:5176:THR:OG1	1:E:5266:GLN:NE2	2.51	0.43
1:F:6102:HIS:CE1	1:F:6103:ARG:HD3	2.54	0.43
1:B:2037:TYR:CD1	1:B:2037:TYR:C	2.97	0.42
1:B:2090:THR:HG22	1:B:2118:ALA:HB3	2.00	0.42
1:C:3170:VAL:HG23	1:C:3173:VAL:HG12	2.01	0.42
1:C:3265:ASN:ND2	1:C:3267:VAL:HB	2.34	0.42
1:A:1220:HIS:O	1:A:1230:HIS:HA	2.18	0.42
1:F:6167:LYS:HE3	1:F:6268:PHE:HD2	1.84	0.42
1:C:3162:ARG:CG	1:C:3162:ARG:NH1	2.83	0.42
1:E:5151:PRO:HB3	1:E:5166:ASN:ND2	2.34	0.42
1:A:1038:THR:HB	1:A:1051:GLY:H	1.84	0.42
1:A:1192:TRP:CE2	1:A:1250:VAL:CG1	3.02	0.42
1:B:2102:HIS:CE1	1:B:2103:ARG:HD3	2.54	0.42
1:B:2265:ASN:ND2	1:B:2267:VAL:HB	2.35	0.42
1:C:3167:LYS:HE3	1:C:3268:PHE:HD2	1.84	0.42
1:D:4091:ILE:HG22	1:D:4100:ILE:CG1	2.48	0.42
1:D:4265:ASN:ND2	1:D:4267:VAL:HB	2.35	0.42
1:A:1091:ILE:HD12	1:A:1117:PHE:HE1	1.84	0.42
1:A:1266:GLN:HG3	1:C:3077:ARG:NH2	2.34	0.42
1:F:6170:VAL:HG23	1:F:6173:VAL:HG12	2.02	0.42
1:A:1057:LYS:HE3	1:A:1057:LYS:HB2	1.85	0.42
1:C:3051:GLY:C	1:C:3052:ILE:HG13	2.45	0.42
1:C:3057:LYS:CG	1:C:3058:THR:H	2.31	0.42
1:E:5162:ARG:CG	1:E:5162:ARG:NH1	2.82	0.42
1:F:6153:THR:O	1:F:6154:LEU:HD12	2.20	0.42
1:F:6162:ARG:CG	1:F:6162:ARG:NH1	2.83	0.42
1:A:1100:ILE:HD13	1:A:1128:PHE:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:ASN:ND2	1:A:1267:VAL:HB	2.34	0.42
1:E:5038:THR:HB	1:E:5051:GLY:H	1.85	0.42
1:F:6003:LEU:HD11	1:F:6039:MET:HG2	2.02	0.42
1:F:6051:GLY:C	1:F:6052:ILE:HG13	2.45	0.42
1:F:6091:ILE:HG22	1:F:6100:ILE:CG1	2.49	0.42
1:F:6265:ASN:ND2	1:F:6267:VAL:HB	2.34	0.42
1:A:1102:HIS:CE1	1:A:1103:ARG:HD3	2.55	0.42
1:A:1151:PRO:HB3	1:A:1166:ASN:ND2	2.34	0.42
1:D:4057:LYS:CG	1:D:4058:THR:H	2.32	0.42
1:D:4151:PRO:HB3	1:D:4166:ASN:ND2	2.35	0.42
1:E:5161:ASN:N	1:E:5161:ASN:ND2	2.68	0.42
1:A:1209:TYR:O	1:A:1236:GLU:N	2.51	0.42
1:B:2192:TRP:CE2	1:B:2250:VAL:HG13	2.54	0.42
1:C:3102:HIS:CE1	1:C:3103:ARG:HG2	2.55	0.42
1:E:5161:ASN:O	1:E:5162:ARG:C	2.63	0.42
1:B:2100:ILE:HD13	1:B:2128:PHE:CE1	2.55	0.41
1:C:3073:TYR:O	1:C:3074:PHE:C	2.63	0.41
1:C:3131:ASN:ND2	1:C:3260:GLY:HA3	2.35	0.41
1:C:3203:ARG:HA	1:C:3203:ARG:HD3	1.89	0.41
1:A:1048:ILE:HD11	1:A:1130:TYR:OH	2.20	0.41
1:B:2091:ILE:HG22	1:B:2100:ILE:CG1	2.50	0.41
1:B:2161:ASN:N	1:B:2161:ASN:ND2	2.68	0.41
1:B:2220:HIS:O	1:B:2230:HIS:HA	2.20	0.41
1:C:3161:ASN:N	1:C:3161:ASN:ND2	2.68	0.41
1:C:3161:ASN:N	1:C:3161:ASN:HD22	2.17	0.41
1:E:5075:LEU:HD12	1:E:5112:ALA:HB3	2.00	0.41
1:E:5152:VAL:HB	1:E:5165:ILE:HG13	2.01	0.41
1:F:6038:THR:HB	1:F:6051:GLY:H	1.85	0.41
1:A:1192:TRP:CH2	1:A:1250:VAL:HG21	2.55	0.41
1:C:3009:ILE:HD11	1:C:3026:PHE:HZ	1.85	0.41
1:C:3100:ILE:HD13	1:C:3128:PHE:CE1	2.55	0.41
1:C:3192:TRP:CH2	1:C:3250:VAL:HG22	2.55	0.41
1:E:5212:MET:HE2	1:E:5235:ASN:N	2.35	0.41
1:B:2057:LYS:HE3	1:B:2057:LYS:HB2	1.85	0.41
1:C:3220:HIS:O	1:C:3230:HIS:HA	2.21	0.41
1:E:5009:ILE:HD11	1:E:5026:PHE:HZ	1.85	0.41
1:E:5210:PHE:HA	1:E:5235:ASN:OD1	2.20	0.41
1:F:6120:ILE:O	1:F:6120:ILE:HG13	2.21	0.41
1:C:3075:LEU:HD12	1:C:3112:ALA:HB3	2.02	0.41
1:C:3182:GLY:HA3	1:C:3259:TRP:CE2	2.55	0.41
1:E:5192:TRP:CE2	1:E:5250:VAL:CG1	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6148:GLU:H	1:F:6148:GLU:HG2	1.51	0.41
1:C:3212:MET:HE1	1:C:3218:VAL:HG23	2.01	0.41
1:F:6161:ASN:O	1:F:6162:ARG:C	2.62	0.41
1:B:2089:GLY:C	1:B:2100:ILE:HD12	2.45	0.41
1:A:1162:ARG:CG	1:A:1162:ARG:NH1	2.84	0.41
1:B:2031:VAL:HG21	1:B:2208:PHE:HE2	1.86	0.41
1:B:2045:ASP:OD2	1:B:2204:MET:HG2	2.21	0.41
1:C:3190:ASN:O	1:C:3191:LEU:HD23	2.21	0.41
1:D:4152:VAL:CG1	1:D:4154:LEU:HD13	2.50	0.41
1:F:6037:TYR:CD1	1:F:6037:TYR:C	2.98	0.41
1:A:1131:ASN:HB2	1:A:1181:MET:SD	2.61	0.41
1:C:3057:LYS:HB2	1:C:3057:LYS:HE3	1.84	0.41
1:C:3205:GLU:HG2	1:C:3261:MET:HB3	2.02	0.41
1:D:4250:VAL:HG11	1:F:6250:VAL:HG11	2.02	0.41
1:E:5087:GLY:HA3	1:E:5124:THR:O	2.21	0.41
1:F:6180:SER:O	1:F:6260:GLY:HA2	2.21	0.41
1:D:4148:GLU:H	1:D:4148:GLU:HG2	1.52	0.40
1:E:5037:TYR:CD1	1:E:5037:TYR:C	3.00	0.40
1:A:1120:ILE:O	1:A:1120:ILE:HG13	2.21	0.40
1:A:1161:ASN:N	1:A:1161:ASN:ND2	2.67	0.40
1:B:2102:HIS:CE1	1:B:2103:ARG:HG2	2.56	0.40
1:B:2161:ASN:O	1:B:2162:ARG:C	2.62	0.40
1:E:5100:ILE:HD13	1:E:5128:PHE:CE1	2.57	0.40
1:E:5211:ASN:CB	1:E:5256:THR:HG23	2.39	0.40
1:A:1007:GLN:HE22	1:C:3011:SER:H	1.70	0.40
1:A:1104:ASP:OD2	1:A:1145:THR:HG22	2.21	0.40
1:A:1161:ASN:O	1:A:1162:ARG:C	2.64	0.40
1:B:2057:LYS:HG2	1:B:2058:THR:O	2.21	0.40
1:D:4120:ILE:O	1:D:4120:ILE:HG13	2.19	0.40
1:D:4162:ARG:HA	1:D:4162:ARG:HD2	1.88	0.40
1:E:5193:ASN:C	1:E:5194:THR:HG1	2.30	0.40
1:B:2078:ARG:HD3	1:B:2132:CYS:SG	2.61	0.40
1:D:4100:ILE:HD12	1:D:4100:ILE:N	2.31	0.40
1:F:6057:LYS:HB2	1:F:6057:LYS:HE3	1.85	0.40
1:F:6185:GLU:HG3	1:F:6256:THR:HB	2.04	0.40
1:A:1192:TRP:CD2	1:A:1250:VAL:HG13	2.57	0.40
1:B:2167:LYS:HE3	1:B:2268:PHE:CD2	2.53	0.40
1:D:4051:GLY:C	1:D:4052:ILE:HG13	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	255/288 (88%)	236 (92%)	16 (6%)	3 (1%)	10	23
1	B	255/288 (88%)	236 (92%)	17 (7%)	2 (1%)	16	34
1	C	255/288 (88%)	236 (92%)	16 (6%)	3 (1%)	10	23
1	D	255/288 (88%)	235 (92%)	16 (6%)	4 (2%)	7	16
1	E	255/288 (88%)	234 (92%)	17 (7%)	4 (2%)	7	16
1	F	255/288 (88%)	236 (92%)	16 (6%)	3 (1%)	10	23
All	All	1530/1728 (88%)	1413 (92%)	98 (6%)	19 (1%)	10	23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1121	ASP
1	A	1162	ARG
1	B	2121	ASP
1	B	2162	ARG
1	C	3121	ASP
1	C	3162	ARG
1	D	4121	ASP
1	D	4162	ARG
1	E	5121	ASP
1	E	5162	ARG
1	F	6121	ASP
1	F	6162	ARG
1	F	6213	ASP
1	A	1213	ASP
1	D	4213	ASP
1	E	5216	ALA
1	C	3213	ASP
1	E	5188	PRO
1	D	4188	PRO

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	221/248 (89%)	201 (91%)	20 (9%)	9	20
1	B	221/248 (89%)	201 (91%)	20 (9%)	9	20
1	C	221/248 (89%)	198 (90%)	23 (10%)	7	14
1	D	221/248 (89%)	199 (90%)	22 (10%)	7	16
1	E	221/248 (89%)	199 (90%)	22 (10%)	7	16
1	F	221/248 (89%)	200 (90%)	21 (10%)	8	18
All	All	1326/1488 (89%)	1198 (90%)	128 (10%)	8	17

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1027	LEU
1	A	1038	THR
1	A	1048	ILE
1	A	1058	THR
1	A	1085	ILE
1	A	1090	THR
1	A	1100	ILE
1	A	1137	THR
1	A	1148	GLU
1	A	1154	LEU
1	A	1157	ASN
1	A	1162	ARG
1	A	1173	VAL
1	A	1193	ASN
1	A	1194	THR
1	A	1213	ASP
1	A	1239	VAL
1	A	1247	HIS
1	A	1250	VAL
1	A	1256	THR
1	B	2027	LEU
1	B	2029	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2048	ILE
1	B	2058	THR
1	B	2085	ILE
1	B	2090	THR
1	B	2100	ILE
1	B	2137	THR
1	B	2148	GLU
1	B	2154	LEU
1	B	2157	ASN
1	B	2162	ARG
1	B	2173	VAL
1	B	2193	ASN
1	B	2194	THR
1	B	2213	ASP
1	B	2239	VAL
1	B	2247	HIS
1	B	2250	VAL
1	B	2256	THR
1	C	3027	LEU
1	C	3029	GLU
1	C	3038	THR
1	C	3048	ILE
1	C	3058	THR
1	C	3085	ILE
1	C	3090	THR
1	C	3100	ILE
1	C	3137	THR
1	C	3148	GLU
1	C	3154	LEU
1	C	3157	ASN
1	C	3162	ARG
1	C	3173	VAL
1	C	3193	ASN
1	C	3194	THR
1	C	3203	ARG
1	C	3204	MET
1	C	3212	MET
1	C	3239	VAL
1	C	3247	HIS
1	C	3250	VAL
1	C	3256	THR
1	D	4027	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4029	GLU
1	D	4038	THR
1	D	4048	ILE
1	D	4058	THR
1	D	4085	ILE
1	D	4090	THR
1	D	4100	ILE
1	D	4137	THR
1	D	4148	GLU
1	D	4154	LEU
1	D	4157	ASN
1	D	4162	ARG
1	D	4173	VAL
1	D	4193	ASN
1	D	4194	THR
1	D	4203	ARG
1	D	4212	MET
1	D	4239	VAL
1	D	4247	HIS
1	D	4250	VAL
1	D	4256	THR
1	E	5027	LEU
1	E	5029	GLU
1	E	5038	THR
1	E	5048	ILE
1	E	5058	THR
1	E	5085	ILE
1	E	5090	THR
1	E	5100	ILE
1	E	5137	THR
1	E	5148	GLU
1	E	5154	LEU
1	E	5157	ASN
1	E	5162	ARG
1	E	5173	VAL
1	E	5193	ASN
1	E	5194	THR
1	E	5203	ARG
1	E	5215	ASP
1	E	5239	VAL
1	E	5247	HIS
1	E	5250	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5256	THR
1	F	6027	LEU
1	F	6029	GLU
1	F	6038	THR
1	F	6048	ILE
1	F	6058	THR
1	F	6085	ILE
1	F	6090	THR
1	F	6100	ILE
1	F	6137	THR
1	F	6148	GLU
1	F	6154	LEU
1	F	6157	ASN
1	F	6162	ARG
1	F	6173	VAL
1	F	6193	ASN
1	F	6194	THR
1	F	6205	GLU
1	F	6239	VAL
1	F	6247	HIS
1	F	6250	VAL
1	F	6256	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1007	GLN
1	A	1020	GLN
1	A	1024	ASN
1	A	1096	GLN
1	A	1102	HIS
1	A	1131	ASN
1	A	1136	HIS
1	A	1157	ASN
1	A	1161	ASN
1	A	1166	ASN
1	A	1193	ASN
1	A	1211	ASN
1	A	1220	HIS
1	B	2007	GLN
1	B	2024	ASN
1	B	2096	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2102	HIS
1	B	2131	ASN
1	B	2157	ASN
1	B	2161	ASN
1	B	2166	ASN
1	B	2193	ASN
1	B	2220	HIS
1	B	2266	GLN
1	C	3007	GLN
1	C	3020	GLN
1	C	3024	ASN
1	C	3096	GLN
1	C	3102	HIS
1	C	3131	ASN
1	C	3136	HIS
1	C	3157	ASN
1	C	3161	ASN
1	C	3166	ASN
1	C	3193	ASN
1	C	3211	ASN
1	C	3220	HIS
1	C	3266	GLN
1	D	4007	GLN
1	D	4024	ASN
1	D	4043	HIS
1	D	4096	GLN
1	D	4102	HIS
1	D	4131	ASN
1	D	4157	ASN
1	D	4161	ASN
1	D	4166	ASN
1	D	4193	ASN
1	D	4211	ASN
1	D	4220	HIS
1	D	4230	HIS
1	D	4266	GLN
1	E	5007	GLN
1	E	5020	GLN
1	E	5024	ASN
1	E	5096	GLN
1	E	5102	HIS
1	E	5131	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5157	ASN
1	E	5161	ASN
1	E	5166	ASN
1	E	5178	GLN
1	E	5193	ASN
1	E	5211	ASN
1	E	5220	HIS
1	E	5266	GLN
1	F	6007	GLN
1	F	6024	ASN
1	F	6096	GLN
1	F	6102	HIS
1	F	6131	ASN
1	F	6157	ASN
1	F	6161	ASN
1	F	6166	ASN
1	F	6193	ASN
1	F	6211	ASN
1	F	6220	HIS
1	F	6230	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/288 (89%)	0.66	33 (12%) 8 6	13, 36, 75, 125	0
1	B	259/288 (89%)	0.69	40 (15%) 5 4	7, 32, 76, 124	0
1	C	259/288 (89%)	0.76	36 (13%) 6 5	10, 38, 83, 130	0
1	D	259/288 (89%)	0.85	45 (17%) 4 3	9, 38, 82, 129	0
1	E	259/288 (89%)	1.30	62 (23%) 2 1	16, 52, 87, 132	0
1	F	259/288 (89%)	1.07	47 (18%) 3 3	19, 45, 85, 129	0
All	All	1554/1728 (89%)	0.89	263 (16%) 4 3	7, 41, 83, 132	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	6254	ALA	7.0
1	F	6263	GLY	6.3
1	F	6188	PRO	6.3
1	B	2193	ASN	6.3
1	D	4263	GLY	6.1
1	C	3263	GLY	6.0
1	E	5268	PHE	5.8
1	E	5158	LEU	5.8
1	B	2263	GLY	5.7
1	D	4264	GLU	5.6
1	B	2158	LEU	5.6
1	D	4158	LEU	5.6
1	B	2267	VAL	5.6
1	D	4188	PRO	5.5
1	E	5155	GLY	5.4
1	F	6268	PHE	5.3
1	A	1265	ASN	5.2
1	B	2268	PHE	5.2
1	A	1268	PHE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1263	GLY	5.1
1	E	5189	GLY	5.0
1	E	5263	GLY	5.0
1	C	3265	ASN	4.9
1	C	3267	VAL	4.9
1	C	3264	GLU	4.9
1	B	2194	THR	4.8
1	D	4155	GLY	4.8
1	D	4161	ASN	4.8
1	E	5188	PRO	4.7
1	B	2172	ASP	4.7
1	B	2265	ASN	4.6
1	F	6193	ASN	4.6
1	E	5162	ARG	4.5
1	C	3193	ASN	4.5
1	C	3268	PHE	4.3
1	D	4246	ILE	4.3
1	B	2161	ASN	4.3
1	A	1158	LEU	4.2
1	F	6158	LEU	4.1
1	E	5194	THR	4.1
1	F	6267	VAL	4.0
1	D	4157	ASN	4.0
1	C	3226	GLN	3.9
1	B	2189	GLY	3.9
1	D	4009	ILE	3.8
1	E	5091	ILE	3.8
1	E	5264	GLU	3.8
1	D	4254	ALA	3.8
1	B	2159	THR	3.8
1	F	6194	THR	3.8
1	D	4268	PHE	3.8
1	E	5265	ASN	3.7
1	E	5187	ALA	3.7
1	B	2067	LYS	3.7
1	A	1193	ASN	3.7
1	A	1194	THR	3.7
1	B	2077	ARG	3.7
1	B	2247	HIS	3.7
1	D	4056	THR	3.6
1	B	2215	ASP	3.6
1	A	1172	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	4156	ASP	3.6
1	E	5193	ASN	3.6
1	E	5267	VAL	3.6
1	A	1247	HIS	3.6
1	D	4193	ASN	3.6
1	D	4203	ARG	3.5
1	F	6265	ASN	3.5
1	F	6155	GLY	3.5
1	F	6136	HIS	3.5
1	A	1267	VAL	3.5
1	E	5118	ALA	3.4
1	C	3158	LEU	3.4
1	C	3247	HIS	3.4
1	C	3067	LYS	3.4
1	C	3194	THR	3.4
1	D	4077	ARG	3.3
1	B	2156	ASP	3.3
1	D	4121	ASP	3.3
1	C	3161	ASN	3.3
1	D	4226	GLN	3.3
1	F	6147	ASP	3.3
1	C	3175	GLU	3.3
1	C	3165	ILE	3.3
1	F	6247	HIS	3.2
1	A	1161	ASN	3.2
1	B	2157	ASN	3.2
1	E	5164	THR	3.2
1	E	5165	ILE	3.2
1	D	4100	ILE	3.1
1	E	5100	ILE	3.1
1	D	4162	ARG	3.1
1	E	5252	THR	3.1
1	E	5120	ILE	3.1
1	F	6243	SER	3.1
1	F	6226	GLN	3.1
1	F	6066	GLY	3.1
1	C	3120	ILE	3.1
1	E	5154	LEU	3.0
1	B	2147	ASP	3.0
1	D	4266	GLN	3.0
1	F	6172	ASP	3.0
1	A	1067	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1012	ALA	3.0
1	B	2120	ILE	3.0
1	F	6100	ILE	3.0
1	E	5160	SER	3.0
1	A	1188	PRO	3.0
1	F	6162	ARG	3.0
1	A	1266	GLN	2.9
1	E	5172	ASP	2.9
1	C	3100	ILE	2.9
1	E	5077	ARG	2.9
1	C	3156	ASP	2.9
1	D	4223	GLY	2.9
1	C	3188	PRO	2.9
1	A	1009	ILE	2.9
1	E	5138	THR	2.9
1	B	2091	ILE	2.9
1	E	5085	ILE	2.9
1	F	6091	ILE	2.9
1	B	2009	ILE	2.8
1	B	2246	ILE	2.8
1	E	5161	ASN	2.8
1	E	5067	LYS	2.8
1	E	5153	THR	2.8
1	F	6246	ILE	2.8
1	D	4265	ASN	2.8
1	B	2056	THR	2.8
1	E	5262	VAL	2.8
1	A	1226	GLN	2.8
1	A	1120	ILE	2.8
1	B	2165	ILE	2.8
1	E	5055	ILE	2.8
1	F	6062	GLY	2.8
1	F	6123	GLY	2.8
1	E	5064	GLU	2.8
1	E	5256	THR	2.8
1	E	5009	ILE	2.7
1	A	1261	MET	2.7
1	C	3152	VAL	2.7
1	E	5137	THR	2.7
1	C	3203	ARG	2.7
1	C	3091	ILE	2.7
1	A	1254	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2137	THR	2.7
1	E	5090	THR	2.7
1	E	5089	GLY	2.7
1	C	3254	ALA	2.7
1	E	5159	THR	2.7
1	F	6189	GLY	2.7
1	B	2254	ALA	2.7
1	C	3121	ASP	2.7
1	E	5246	ILE	2.6
1	C	3064	GLU	2.6
1	E	5157	ASN	2.6
1	A	1137	THR	2.6
1	A	1246	ILE	2.6
1	D	4120	ILE	2.6
1	B	2136	HIS	2.6
1	E	5136	HIS	2.6
1	A	1100	ILE	2.6
1	D	4189	GLY	2.6
1	E	5190	ASN	2.6
1	E	5247	HIS	2.5
1	C	3262	VAL	2.5
1	E	5266	GLN	2.5
1	A	1121	ASP	2.5
1	D	4172	ASP	2.5
1	E	5103	ARG	2.5
1	D	4007	GLN	2.5
1	E	5226	GLN	2.5
1	E	5254	ALA	2.5
1	F	6150	SER	2.5
1	D	4091	ILE	2.5
1	E	5156	ASP	2.5
1	F	6067	LYS	2.5
1	F	6163	ARG	2.5
1	B	2226	GLN	2.5
1	C	3252	THR	2.5
1	D	4194	THR	2.5
1	A	1091	ILE	2.5
1	C	3009	ILE	2.5
1	D	4002	SER	2.5
1	E	5180	SER	2.5
1	A	1189	GLY	2.5
1	E	5135	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	3162	ARG	2.4
1	F	6077	ARG	2.4
1	F	6148	GLU	2.4
1	A	1065	VAL	2.4
1	B	2266	GLN	2.4
1	B	2162	ARG	2.4
1	D	4229	ARG	2.4
1	C	3136	HIS	2.4
1	C	3147	ASP	2.4
1	C	3172	ASP	2.4
1	F	6073	TYR	2.4
1	C	3077	ARG	2.4
1	B	2190	ASN	2.4
1	A	1243	SER	2.4
1	B	2188	PRO	2.4
1	D	4067	LYS	2.4
1	F	6152	VAL	2.4
1	F	6037	TYR	2.4
1	D	4138	THR	2.4
1	A	1147	ASP	2.4
1	E	5142	LYS	2.4
1	E	5152	VAL	2.4
1	D	4247	HIS	2.3
1	E	5185	GLU	2.3
1	A	1007	GLN	2.3
1	A	1077	ARG	2.3
1	D	4147	ASP	2.3
1	F	6007	GLN	2.3
1	C	3137	THR	2.3
1	F	6137	THR	2.3
1	F	6161	ASN	2.3
1	B	2163	ARG	2.3
1	F	6069	LEU	2.3
1	F	6154	LEU	2.3
1	F	6191	LEU	2.3
1	B	2100	ILE	2.2
1	D	4064	GLU	2.2
1	B	2002	SER	2.2
1	D	4215	ASP	2.2
1	D	4241	SER	2.2
1	E	5150	SER	2.2
1	D	4262	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	5178	GLN	2.2
1	B	2155	GLY	2.2
1	E	5215	ASP	2.2
1	A	1085	ILE	2.2
1	B	2029	GLU	2.2
1	C	3057	LYS	2.2
1	F	6072	SER	2.2
1	F	6187	ALA	2.2
1	B	2148	GLU	2.2
1	C	3266	GLN	2.2
1	D	4224	GLN	2.2
1	F	6266	GLN	2.2
1	E	5191	LEU	2.2
1	C	3246	ILE	2.2
1	F	6092	THR	2.1
1	D	4253	LYS	2.1
1	F	6009	ILE	2.1
1	E	5148	GLU	2.1
1	F	6252	THR	2.1
1	F	6121	ASP	2.1
1	F	6261	MET	2.1
1	E	5203	ARG	2.1
1	E	5192	TRP	2.1
1	E	5141	THR	2.1
1	F	6190	ASN	2.1
1	A	1165	ILE	2.1
1	B	2046	ARG	2.0
1	E	5175	GLU	2.0
1	D	4090	THR	2.0
1	D	4165	ILE	2.0
1	D	4046	ARG	2.0
1	A	1215	ASP	2.0
1	B	2085	ILE	2.0
1	D	4101	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.