Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:37 am BST

PDB ID	:	1OU5
Title	:	Crystal structure of human CCA-adding enzyme
Authors	:	Augustin, M.A.; Reichert, A.S.; Betat, H.; Huber, R.; Moerl, M.; Steegborn, C.
Deposited on	:	2003-03-24
Resolution	:	3.40 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:

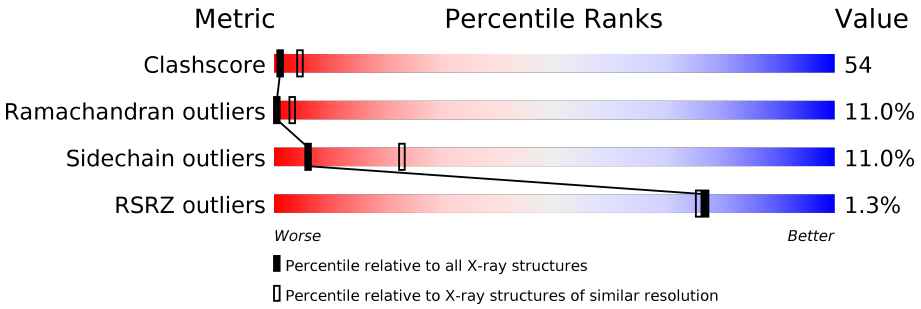
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	448	% 27% 38% 11% 23%
1	B	448	% 27% 39% 10% 23%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5570 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 tRNA CCA-adding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	266	0	0
			2785	1776	480	521	8			
1	B	344	Total	C	N	O	S	194	0	0
			2785	1776	480	521	8			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	CLONING ARTIFACT	UNP Q96Q11
A	-41	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-40	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-39	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-38	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-37	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-36	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-35	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-34	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-33	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-32	LEU	-	CLONING ARTIFACT	UNP Q96Q11
A	-31	VAL	-	CLONING ARTIFACT	UNP Q96Q11
A	-30	PRO	-	CLONING ARTIFACT	UNP Q96Q11
A	-29	ARG	-	CLONING ARTIFACT	UNP Q96Q11
A	-28	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-27	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-26	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-25	MET	-	CLONING ARTIFACT	UNP Q96Q11
A	-24	LYS	-	CLONING ARTIFACT	UNP Q96Q11
A	-23	GLU	-	CLONING ARTIFACT	UNP Q96Q11
A	-22	THR	-	CLONING ARTIFACT	UNP Q96Q11
A	-21	ALA	-	CLONING ARTIFACT	UNP Q96Q11
A	-20	ALA	-	CLONING ARTIFACT	UNP Q96Q11
A	-19	ALA	-	CLONING ARTIFACT	UNP Q96Q11
A	-18	LYS	-	CLONING ARTIFACT	UNP Q96Q11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	PHE	-	CLONING ARTIFACT	UNP Q96Q11
A	-16	GLU	-	CLONING ARTIFACT	UNP Q96Q11
A	-15	ARG	-	CLONING ARTIFACT	UNP Q96Q11
A	-14	GLN	-	CLONING ARTIFACT	UNP Q96Q11
A	-13	HIS	-	CLONING ARTIFACT	UNP Q96Q11
A	-12	MET	-	CLONING ARTIFACT	UNP Q96Q11
A	-11	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-10	SER	-	CLONING ARTIFACT	UNP Q96Q11
A	-9	PRO	-	CLONING ARTIFACT	UNP Q96Q11
A	-8	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-7	LEU	-	CLONING ARTIFACT	UNP Q96Q11
A	-6	GLY	-	CLONING ARTIFACT	UNP Q96Q11
A	-5	THR	-	CLONING ARTIFACT	UNP Q96Q11
A	-4	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-3	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-2	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	-1	ASP	-	CLONING ARTIFACT	UNP Q96Q11
A	0	LYS	-	CLONING ARTIFACT	UNP Q96Q11
B	-42	MET	-	CLONING ARTIFACT	UNP Q96Q11
B	-41	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-40	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-39	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-38	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-37	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-36	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-35	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-34	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-33	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-32	LEU	-	CLONING ARTIFACT	UNP Q96Q11
B	-31	VAL	-	CLONING ARTIFACT	UNP Q96Q11
B	-30	PRO	-	CLONING ARTIFACT	UNP Q96Q11
B	-29	ARG	-	CLONING ARTIFACT	UNP Q96Q11
B	-28	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-27	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-26	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-25	MET	-	CLONING ARTIFACT	UNP Q96Q11
B	-24	LYS	-	CLONING ARTIFACT	UNP Q96Q11
B	-23	GLU	-	CLONING ARTIFACT	UNP Q96Q11
B	-22	THR	-	CLONING ARTIFACT	UNP Q96Q11
B	-21	ALA	-	CLONING ARTIFACT	UNP Q96Q11
B	-20	ALA	-	CLONING ARTIFACT	UNP Q96Q11
B	-19	ALA	-	CLONING ARTIFACT	UNP Q96Q11

Continued on next page...

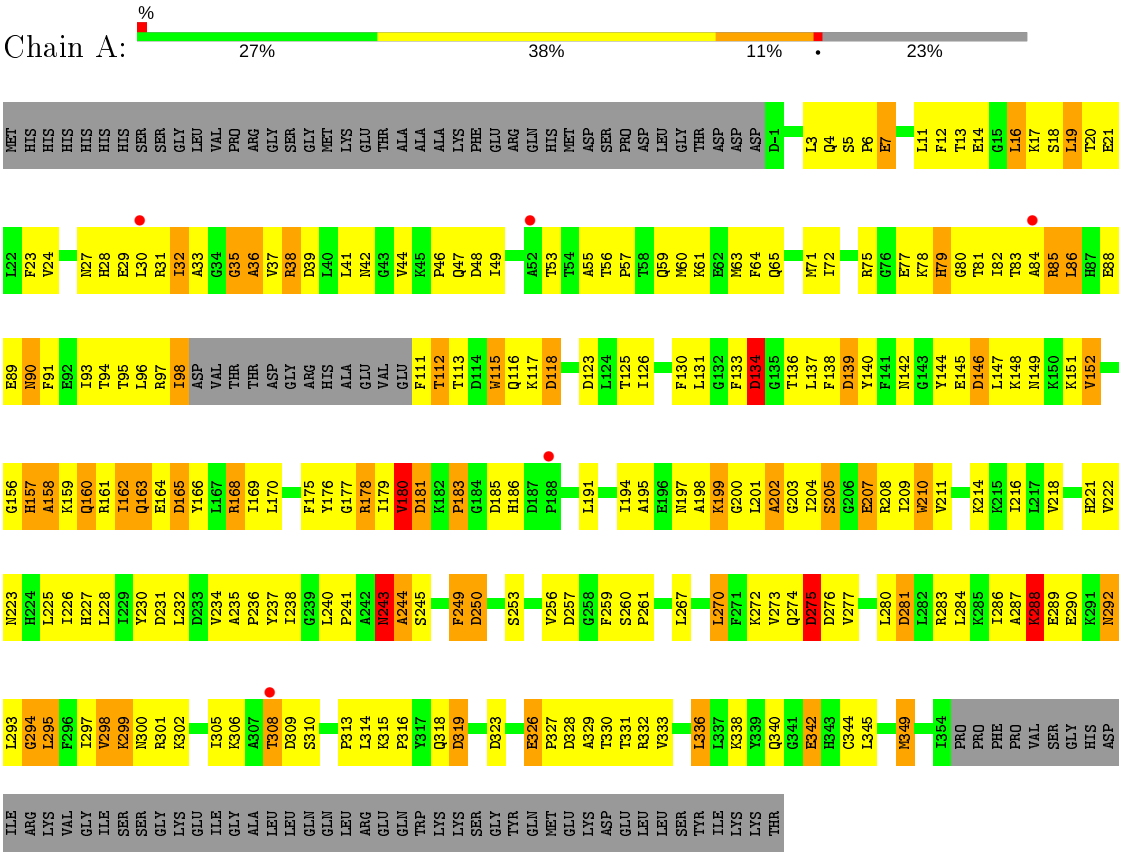
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	CLONING ARTIFACT	UNP Q96Q11
B	-17	PHE	-	CLONING ARTIFACT	UNP Q96Q11
B	-16	GLU	-	CLONING ARTIFACT	UNP Q96Q11
B	-15	ARG	-	CLONING ARTIFACT	UNP Q96Q11
B	-14	GLN	-	CLONING ARTIFACT	UNP Q96Q11
B	-13	HIS	-	CLONING ARTIFACT	UNP Q96Q11
B	-12	MET	-	CLONING ARTIFACT	UNP Q96Q11
B	-11	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-10	SER	-	CLONING ARTIFACT	UNP Q96Q11
B	-9	PRO	-	CLONING ARTIFACT	UNP Q96Q11
B	-8	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-7	LEU	-	CLONING ARTIFACT	UNP Q96Q11
B	-6	GLY	-	CLONING ARTIFACT	UNP Q96Q11
B	-5	THR	-	CLONING ARTIFACT	UNP Q96Q11
B	-4	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-3	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-2	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	-1	ASP	-	CLONING ARTIFACT	UNP Q96Q11
B	0	LYS	-	CLONING ARTIFACT	UNP Q96Q11

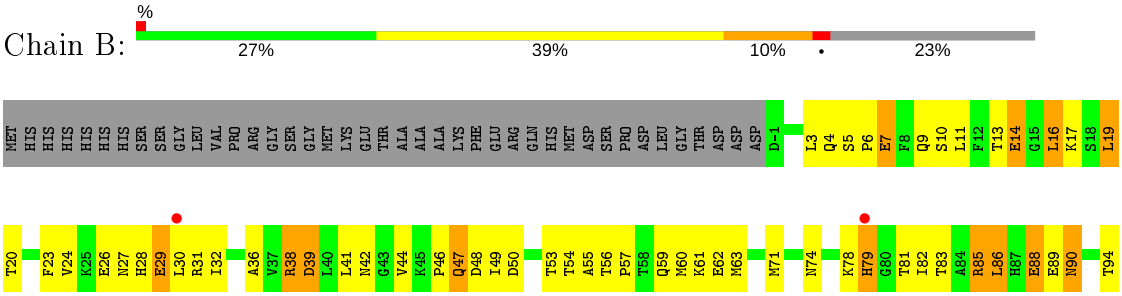
3 Residue-property plots (i)

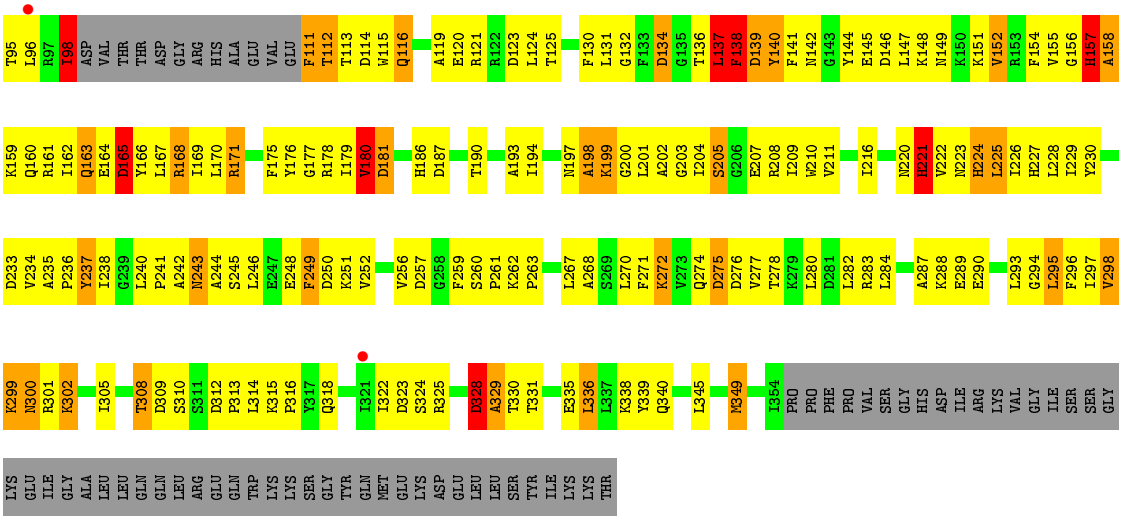
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 1: tRNA CCA-adding enzyme




T95 L96 R97 I98 ASP VAL THR THR ASP GLY ARG HIS ALA GLU VAL GLU F111 T112 T113 D114 W115 Q116 A119 E120 R121 R122 D123 L124 T125 F130 L131 G132 F133 D134 G135 T136 L137 F138 D139 Y140 F141 N142 G143 Y144 E145 D146 L147 K148 N149 K150 K151 V152 R153 F154 V155 G156 H157 A158
K159 Q160 R161 I162 Q163 E164 D165 Y166 L167 R168 I169 L170 R171 F175 Y176 G177 R178 I179 V180 D181 H186 D187 T190 A193 I194 N197 A198 K199 G200 L201 A202 G203 I204 S205 G206 E207 R208 I209 W210 V211 I216 N220 H221 V222 N223 H224 L225 I226 H227 L228 I229 Y230
D233 V234 A235 P236 Y237 I238 G239 L240 P241 A242 N243 A244 S245 L246 E247 E248 F249 D250 K251 V252 V256 D257 G258 F259 S260 P261 K262 P263 L267 A268 S269 L270 F271 K272 V273 Q274 D275 D276 V277 T278 K279 L280 D281 L282 R283 L284 A287 K288 E289 E290 L293 G294 L295 F296 I297 V298
K299 N300 R301 K302 I305 T308 D309 S310 S311 D312 P313 L314 K315 P316 Y317 Q318 I321 I322 D323 S324 R325 D328 A329 T330 T331 E335 L336 L337 K338 Y339 Q340 L345 M349 I354 PRO PRO PHE PRO VAL SER GLY HIS ASP ILE ARG LYS VAL GLY ILE SER SER GLY
LYS GLU ILE GLY ALA LEU LEU GLN GLN LEU ARG GLU GLN TRP LYS LYS SER GLY TYR GLN MET GLU LYS ASP GLU LEU LEU SER TYR ILE LYS LYS THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.52Å 102.52Å 206.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.40 44.65 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.40) 98.3 (44.65-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.278 , 0.318 0.295 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	86.0	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5570	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.78	5/2839 (0.2%)	1.02	21/3826 (0.5%)
1	B	0.61	1/2839 (0.0%)	0.95	16/3826 (0.4%)
All	All	0.70	6/5678 (0.1%)	0.99	37/7652 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ILE	C-N	22.89	1.86	1.34
1	B	98	ILE	CB-CG2	12.08	1.90	1.52
1	A	98	ILE	CB-CG2	8.71	1.79	1.52
1	A	342	GLU	CG-CD	7.60	1.63	1.51
1	A	98	ILE	CA-C	5.91	1.68	1.52
1	A	98	ILE	CB-CG1	-5.79	1.37	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ILE	N-CA-C	-10.57	82.46	111.00
1	B	111	PHE	N-CA-CB	9.77	128.19	110.60
1	A	98	ILE	CA-C-N	9.36	137.80	117.20
1	A	98	ILE	N-CA-C	-9.33	85.80	111.00
1	B	98	ILE	CG1-CB-CG2	-9.10	91.38	111.40
1	A	98	ILE	C-N-CA	-7.64	102.60	121.70
1	B	137	LEU	CB-CA-C	-7.33	96.27	110.20
1	A	98	ILE	O-C-N	-7.24	111.11	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	GLY	N-CA-C	-7.19	95.13	113.10
1	A	231	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	98	ILE	CA-CB-CG1	6.51	123.37	111.00
1	B	137	LEU	CB-CG-CD1	-6.26	100.36	111.00
1	B	257	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	288	LYS	CD-CE-NZ	5.88	125.22	111.70
1	A	275	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	187	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	98	ILE	CA-CB-CG2	-5.76	99.38	110.90
1	B	120	GLU	N-CA-C	-5.63	95.80	111.00
1	A	98	ILE	CA-CB-CG2	-5.56	99.78	110.90
1	A	118	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	319	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	134	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	323	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	139	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	138	PHE	CB-CG-CD1	-5.35	117.05	120.80
1	A	281	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	39	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	97	ARG	C-N-CA	5.25	134.83	121.70
1	A	146	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	250	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	50	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	139	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	180	VAL	CB-CA-C	-5.01	101.88	111.40
1	B	328	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	114	ASP	CB-CG-OD2	5.00	122.80	118.30
1	A	257	ASP	CB-CG-OD2	5.00	122.80	118.30
1	A	288	LYS	N-CA-CB	-5.00	101.60	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	98	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2785	0	2799	252	1
1	B	2785	0	2803	286	1
All	All	5570	0	5602	537	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 54.

All (537) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:HA	1:B:237:TYR:CE1	1.46	1.45
1:B:199:LYS:HA	1:B:237:TYR:CD1	1.69	1.24
1:B:241:PRO:HG3	1:B:271:PHE:HB3	1.35	1.06
1:B:209:ILE:HD11	1:B:284:LEU:HD11	1.34	1.05
1:B:199:LYS:CA	1:B:237:TYR:CE1	2.39	1.05
1:B:314:LEU:HD11	1:B:349:MET:HG2	1.42	1.01
1:A:308:THR:HG22	1:A:310:SER:H	1.25	0.98
1:B:131:LEU:HD23	1:B:136:THR:O	1.66	0.96
1:A:226:ILE:HG12	1:A:249:PHE:CZ	2.00	0.96
1:B:237:TYR:HD2	1:B:237:TYR:N	1.64	0.95
1:B:308:THR:O	1:B:309:ASP:CG	2.06	0.93
1:B:236:PRO:HG2	1:B:237:TYR:CD2	2.04	0.92
1:B:199:LYS:CA	1:B:237:TYR:HE1	1.80	0.91
1:B:119:ALA:O	1:B:141:PHE:CE2	2.24	0.90
1:A:230:TYR:CD2	1:A:243:ASN:HB3	2.06	0.90
1:A:209:ILE:HD11	1:A:284:LEU:HD11	1.52	0.90
1:B:272:LYS:HE2	1:B:299:LYS:H	1.35	0.90
1:B:199:LYS:HA	1:B:237:TYR:HE1	1.11	0.89
1:A:32:ILE:HD11	1:A:36:ALA:O	1.72	0.89
1:B:308:THR:HG22	1:B:310:SER:H	1.39	0.88
1:B:274:GLN:O	1:B:275:ASP:HB3	1.74	0.87
1:B:199:LYS:CA	1:B:237:TYR:CD1	2.57	0.87
1:B:267:LEU:O	1:B:270:LEU:HD23	1.75	0.86
1:A:336:LEU:HD22	1:A:340:GLN:HG3	1.55	0.86
1:B:119:ALA:O	1:B:141:PHE:HE2	1.56	0.85
1:B:226:ILE:HG12	1:B:249:PHE:CZ	2.12	0.84
1:B:237:TYR:N	1:B:237:TYR:CD2	2.39	0.83
1:B:179:ILE:O	1:B:180:VAL:HG13	1.77	0.83
1:B:275:ASP:H	1:B:277:VAL:HG12	1.43	0.83
1:B:146:ASP:HB3	1:B:151:LYS:HB3	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:O	1:A:24:VAL:HG23	1.79	0.82
1:A:301:ARG:O	1:A:305:ILE:HG22	1.78	0.82
1:B:336:LEU:HD22	1:B:340:GLN:HG3	1.61	0.81
1:B:165:ASP:HB3	1:B:168:ARG:HD3	1.63	0.80
1:B:280:LEU:HD11	1:B:284:LEU:HD22	1.64	0.80
1:A:280:LEU:HD11	1:A:284:LEU:HD22	1.64	0.79
1:A:39:ASP:HB3	1:A:44:VAL:HG23	1.65	0.79
1:B:46:PRO:HB2	1:B:49:ILE:HG12	1.64	0.79
1:B:197:ASN:O	1:B:198:ALA:HB3	1.81	0.78
1:B:272:LYS:HE2	1:B:299:LYS:N	1.98	0.78
1:B:236:PRO:HG2	1:B:237:TYR:CE2	2.18	0.78
1:B:11:LEU:HD11	1:B:46:PRO:HG3	1.65	0.77
1:B:199:LYS:CB	1:B:237:TYR:HE1	1.97	0.77
1:B:315:LYS:N	1:B:316:PRO:HD2	2.00	0.77
1:A:19:LEU:HD12	1:A:91:PHE:CD2	2.18	0.77
1:A:35:GLY:O	1:A:36:ALA:CB	2.30	0.76
1:B:165:ASP:HB3	1:B:168:ARG:CD	2.16	0.76
1:A:274:GLN:O	1:A:275:ASP:HB2	1.84	0.76
1:B:20:THR:O	1:B:24:VAL:HG23	1.86	0.76
1:A:46:PRO:HB2	1:A:49:ILE:HG12	1.68	0.75
1:A:230:TYR:CE2	1:A:243:ASN:HB3	2.22	0.74
1:A:160:GLN:HA	1:A:163:GLN:HB3	1.69	0.74
1:A:197:ASN:O	1:A:198:ALA:HB3	1.87	0.73
1:A:314:LEU:HD11	1:A:349:MET:HG2	1.69	0.73
1:B:298:VAL:O	1:B:300:ASN:N	2.20	0.73
1:A:160:GLN:HA	1:A:163:GLN:CB	2.19	0.73
1:B:274:GLN:O	1:B:275:ASP:CB	2.37	0.73
1:A:126:ILE:HD12	1:A:147:LEU:HB2	1.71	0.73
1:B:300:ASN:O	1:B:301:ARG:HD3	1.89	0.72
1:B:260:SER:H	1:B:338:LYS:NZ	1.87	0.72
1:A:130:PHE:HB2	1:A:138:PHE:HB2	1.71	0.72
1:A:146:ASP:HB3	1:A:151:LYS:HB3	1.70	0.72
1:A:178:ARG:CG	1:A:178:ARG:HH21	2.02	0.71
1:A:147:LEU:O	1:A:148:LYS:HB3	1.90	0.71
1:B:145:GLU:O	1:B:149:ASN:HB2	1.91	0.71
1:A:287:ALA:O	1:A:290:GLU:HB2	1.89	0.71
1:B:11:LEU:HD22	1:B:49:ILE:HD11	1.72	0.71
1:A:170:LEU:HD11	1:A:238:ILE:HD11	1.71	0.71
1:A:336:LEU:HD13	1:A:340:GLN:NE2	2.05	0.70
1:A:11:LEU:HD22	1:A:49:ILE:HD11	1.74	0.70
1:B:260:SER:H	1:B:338:LYS:HZ1	1.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:THR:HG22	1:A:310:SER:N	2.04	0.69
1:A:95:THR:HG21	1:A:112:THR:HG23	1.73	0.69
1:B:209:ILE:HD12	1:B:238:ILE:HG13	1.73	0.69
1:A:165:ASP:O	1:A:168:ARG:HD3	1.92	0.69
1:A:56:THR:OG1	1:A:59:GLN:HG2	1.91	0.69
1:A:41:LEU:HD13	1:A:144:TYR:HD1	1.56	0.69
1:B:157:HIS:C	1:B:159:LYS:H	1.96	0.68
1:A:147:LEU:C	1:A:149:ASN:H	1.97	0.68
1:B:111:PHE:O	1:B:113:THR:N	2.27	0.68
1:A:61:LYS:HA	1:A:71:MET:HE1	1.75	0.68
1:B:95:THR:HG21	1:B:112:THR:HG23	1.75	0.68
1:A:288:LYS:O	1:A:290:GLU:N	2.24	0.67
1:B:205:SER:HB3	1:B:208:ARG:HB3	1.74	0.67
1:B:299:LYS:O	1:B:300:ASN:C	2.33	0.67
1:A:230:TYR:HD2	1:A:243:ASN:HB3	1.53	0.67
1:A:178:ARG:HH21	1:A:178:ARG:HG3	1.60	0.67
1:B:237:TYR:HD2	1:B:237:TYR:H	1.39	0.67
1:A:210:TRP:CE3	1:A:284:LEU:HD23	2.29	0.67
1:A:315:LYS:N	1:A:316:PRO:HD2	2.10	0.67
1:B:42:ASN:HD21	1:B:147:LEU:HD11	1.58	0.67
1:B:56:THR:OG1	1:B:59:GLN:HG2	1.95	0.67
1:A:299:LYS:HA	1:A:302:LYS:HB3	1.77	0.67
1:B:151:LYS:O	1:B:152:VAL:HB	1.93	0.66
1:B:130:PHE:O	1:B:137:LEU:O	2.14	0.66
1:B:305:ILE:O	1:B:305:ILE:HG23	1.94	0.66
1:A:305:ILE:HG23	1:A:305:ILE:O	1.94	0.66
1:A:89:GLU:O	1:A:90:ASN:HB2	1.96	0.65
1:A:11:LEU:HD11	1:A:46:PRO:HG3	1.78	0.65
1:B:31:ARG:CZ	1:B:116:GLN:OE1	2.44	0.65
1:A:139:ASP:O	1:A:140:TYR:HB2	1.97	0.65
1:A:273:VAL:O	1:A:276:ASP:HB3	1.97	0.65
1:B:301:ARG:O	1:B:305:ILE:HG22	1.96	0.65
1:A:11:LEU:O	1:A:16:LEU:HD12	1.97	0.65
1:B:160:GLN:O	1:B:163:GLN:HB3	1.97	0.65
1:A:145:GLU:O	1:A:149:ASN:HB2	1.97	0.65
1:B:226:ILE:HD12	1:B:227:HIS:N	2.11	0.65
1:A:273:VAL:HG12	1:A:274:GLN:N	2.12	0.64
1:B:283:ARG:HG3	1:B:284:LEU:CD1	2.27	0.64
1:B:39:ASP:HB3	1:B:44:VAL:HG23	1.78	0.64
1:B:197:ASN:O	1:B:198:ALA:CB	2.45	0.64
1:A:115:TRP:O	1:A:117:LYS:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HD3	1:B:116:GLN:HE22	1.61	0.64
1:B:61:LYS:C	1:B:63:MET:H	1.99	0.64
1:A:134:ASP:OD2	1:A:136:THR:OG1	2.13	0.63
1:A:32:ILE:HG22	1:A:133:PHE:HE2	1.63	0.63
1:A:151:LYS:O	1:A:152:VAL:HB	1.98	0.63
1:A:259:PHE:CD1	1:A:259:PHE:N	2.66	0.63
1:B:180:VAL:O	1:B:181:ASP:CB	2.45	0.63
1:B:166:TYR:CD2	1:B:200:GLY:HA3	2.34	0.63
1:B:60:MET:O	1:B:63:MET:HB3	1.99	0.63
1:B:210:TRP:CE3	1:B:284:LEU:HD23	2.33	0.63
1:A:35:GLY:O	1:A:36:ALA:HB3	1.98	0.63
1:B:158:ALA:HB3	1:B:193:ALA:CB	2.29	0.63
1:B:165:ASP:O	1:B:168:ARG:HD3	1.98	0.62
1:B:205:SER:HB3	1:B:208:ARG:CB	2.28	0.62
1:B:78:LYS:O	1:B:79:HIS:O	2.16	0.62
1:A:111:PHE:O	1:A:113:THR:N	2.32	0.62
1:A:308:THR:O	1:A:309:ASP:HB2	1.99	0.62
1:B:280:LEU:CD1	1:B:284:LEU:HD22	2.30	0.62
1:B:53:THR:O	1:B:95:THR:HA	2.00	0.62
1:B:160:GLN:HA	1:B:163:GLN:HB3	1.81	0.62
1:B:124:LEU:HD23	1:B:154:PHE:HA	1.82	0.61
1:A:201:LEU:HD12	1:A:234:VAL:HG13	1.82	0.61
1:B:23:PHE:CD2	1:B:30:LEU:HD12	2.34	0.61
1:B:308:THR:HG22	1:B:310:SER:N	2.14	0.61
1:A:158:ALA:C	1:A:160:GLN:H	2.01	0.61
1:B:201:LEU:HD13	1:B:238:ILE:HD13	1.82	0.61
1:A:160:GLN:O	1:A:163:GLN:HB3	2.01	0.61
1:A:160:GLN:CA	1:A:163:GLN:HB3	2.31	0.61
1:B:275:ASP:N	1:B:277:VAL:HG12	2.14	0.61
1:B:328:ASP:O	1:B:329:ALA:C	2.37	0.61
1:A:126:ILE:CD1	1:A:147:LEU:HB2	2.29	0.61
1:B:30:LEU:C	1:B:30:LEU:HD23	2.20	0.61
1:B:308:THR:OG1	1:B:313:PRO:HA	2.01	0.61
1:B:299:LYS:O	1:B:301:ARG:N	2.34	0.61
1:A:216:ILE:HG23	1:A:225:LEU:HD13	1.83	0.60
1:B:147:LEU:C	1:B:149:ASN:H	2.04	0.60
1:A:166:TYR:CD2	1:A:200:GLY:HA3	2.36	0.60
1:A:23:PHE:CD2	1:A:30:LEU:HD12	2.37	0.60
1:A:280:LEU:CD1	1:A:284:LEU:HD22	2.30	0.60
1:A:294:GLY:O	1:A:298:VAL:HG23	2.02	0.60
1:A:125:THR:HG21	1:A:146:ASP:OD1	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ALA:O	1:A:333:VAL:HG23	2.00	0.60
1:A:292:ASN:HA	1:A:295:LEU:HD21	1.84	0.60
1:A:336:LEU:HD22	1:A:340:GLN:CG	2.28	0.60
1:A:82:ILE:O	1:A:93:ILE:N	2.31	0.60
1:B:158:ALA:C	1:B:160:GLN:H	2.02	0.60
1:A:328:ASP:O	1:A:329:ALA:C	2.40	0.59
1:B:236:PRO:CG	1:B:237:TYR:CE2	2.85	0.59
1:A:11:LEU:HD21	1:A:46:PRO:HG2	1.84	0.59
1:A:209:ILE:HD12	1:A:238:ILE:CD1	2.31	0.59
1:B:11:LEU:HD21	1:B:46:PRO:HG2	1.84	0.59
1:B:308:THR:O	1:B:309:ASP:OD1	2.18	0.59
1:A:179:ILE:O	1:A:180:VAL:HG13	2.02	0.59
1:A:30:LEU:C	1:A:30:LEU:HD23	2.23	0.59
1:A:197:ASN:O	1:A:198:ALA:CB	2.51	0.59
1:A:201:LEU:HD13	1:A:238:ILE:HD13	1.84	0.59
1:A:72:ILE:HD11	1:A:90:ASN:ND2	2.18	0.59
1:A:41:LEU:HD13	1:A:144:TYR:CD1	2.37	0.58
1:A:275:ASP:C	1:A:277:VAL:H	2.05	0.58
1:A:226:ILE:HD12	1:A:227:HIS:N	2.17	0.58
1:A:299:LYS:C	1:A:301:ARG:N	2.56	0.58
1:B:11:LEU:O	1:B:13:THR:HG23	2.04	0.58
1:B:82:ILE:HG22	1:B:83:THR:N	2.18	0.58
1:A:300:ASN:O	1:A:301:ARG:HD3	2.04	0.57
1:A:64:PHE:HB2	1:A:71:MET:HE1	1.86	0.57
1:A:96:LEU:HD12	1:A:96:LEU:H	1.68	0.57
1:B:283:ARG:HG3	1:B:284:LEU:HD12	1.85	0.57
1:B:31:ARG:NH2	1:B:116:GLN:HE22	2.02	0.57
1:B:209:ILE:HD11	1:B:284:LEU:CD1	2.22	0.57
1:A:85:ARG:HG2	1:A:90:ASN:ND2	2.19	0.57
1:A:162:ILE:O	1:A:164:GLU:N	2.38	0.57
1:B:180:VAL:O	1:B:181:ASP:HB2	2.02	0.57
1:A:11:LEU:HD21	1:A:46:PRO:CG	2.34	0.57
1:B:235:ALA:N	1:B:236:PRO:HD2	2.19	0.57
1:B:289:GLU:O	1:B:293:LEU:N	2.34	0.57
1:B:335:GLU:OE1	1:B:338:LYS:HE3	2.05	0.57
1:A:315:LYS:HA	1:A:318:GLN:HE21	1.70	0.57
1:B:199:LYS:HA	1:B:237:TYR:HD1	1.58	0.57
1:B:256:VAL:HB	1:B:261:PRO:HB3	1.87	0.57
1:B:28:HIS:CG	1:B:55:ALA:HB2	2.39	0.57
1:B:157:HIS:O	1:B:159:LYS:N	2.38	0.56
1:B:259:PHE:N	1:B:259:PHE:CD1	2.72	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLU:HG2	1:B:63:MET:HE2	1.87	0.56
1:A:186:HIS:HB3	1:A:191:LEU:HD13	1.87	0.56
1:A:61:LYS:C	1:A:63:MET:H	2.07	0.56
1:A:205:SER:HB3	1:A:208:ARG:CB	2.36	0.56
1:B:139:ASP:O	1:B:140:TYR:HB2	2.04	0.56
1:B:313:PRO:O	1:B:314:LEU:HB3	2.05	0.56
1:A:227:HIS:HE1	1:A:250:ASP:OD2	1.89	0.56
1:A:293:LEU:O	1:A:293:LEU:HD12	2.06	0.56
1:B:242:ALA:O	1:B:243:ASN:C	2.42	0.56
1:B:30:LEU:HD23	1:B:31:ARG:N	2.21	0.56
1:A:297:ILE:O	1:A:299:LYS:N	2.39	0.56
1:B:85:ARG:HD3	1:B:88:GLU:HA	1.88	0.55
1:A:78:LYS:O	1:A:79:HIS:CB	2.55	0.55
1:A:230:TYR:HE1	1:A:240:LEU:HD13	1.69	0.55
1:A:85:ARG:HE	1:A:90:ASN:ND2	2.05	0.55
1:B:96:LEU:H	1:B:96:LEU:HD12	1.71	0.55
1:B:216:ILE:HG23	1:B:225:LEU:HD13	1.89	0.55
1:A:199:LYS:HA	1:A:237:TYR:CE1	2.42	0.55
1:B:98:ILE:O	1:B:111:PHE:HD1	1.90	0.55
1:B:132:GLY:C	1:B:134:ASP:H	2.10	0.55
1:B:288:LYS:O	1:B:289:GLU:HB3	2.06	0.55
1:A:147:LEU:C	1:A:149:ASN:N	2.60	0.55
1:A:283:ARG:HG3	1:A:284:LEU:CD1	2.37	0.55
1:B:146:ASP:CB	1:B:151:LYS:HB3	2.33	0.54
1:B:274:GLN:HG3	1:B:295:LEU:HB3	1.90	0.54
1:A:160:GLN:HA	1:A:163:GLN:HB2	1.89	0.54
1:B:223:ASN:HA	1:B:249:PHE:HE2	1.71	0.54
1:B:315:LYS:N	1:B:316:PRO:CD	2.70	0.54
1:A:81:THR:HG23	1:A:94:THR:OG1	2.07	0.54
1:B:160:GLN:HA	1:B:163:GLN:CB	2.37	0.54
1:B:241:PRO:HG3	1:B:271:PHE:CB	2.22	0.54
1:B:260:SER:N	1:B:338:LYS:NZ	2.55	0.54
1:B:38:ARG:HG2	1:B:38:ARG:HH21	1.73	0.54
1:B:157:HIS:C	1:B:159:LYS:N	2.61	0.53
1:B:163:GLN:O	1:B:163:GLN:HG2	2.08	0.53
1:B:299:LYS:C	1:B:301:ARG:N	2.61	0.53
1:B:336:LEU:HD22	1:B:340:GLN:HE21	1.74	0.53
1:A:164:GLU:O	1:A:165:ASP:C	2.46	0.53
1:B:119:ALA:O	1:B:141:PHE:CZ	2.62	0.53
1:A:210:TRP:NE1	1:A:286:ILE:HG22	2.24	0.53
1:B:175:PHE:C	1:B:177:GLY:N	2.59	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:O	1:A:181:ASP:CB	2.56	0.53
1:A:256:VAL:HB	1:A:261:PRO:HB3	1.91	0.53
1:A:259:PHE:H	1:A:259:PHE:HD1	1.54	0.53
1:A:30:LEU:HD23	1:A:31:ARG:N	2.24	0.53
1:A:84:ALA:O	1:A:90:ASN:HA	2.08	0.53
1:A:165:ASP:HB3	1:A:168:ARG:HD3	1.90	0.53
1:A:250:ASP:O	1:A:253:SER:HB3	2.08	0.53
1:A:288:LYS:O	1:A:289:GLU:HB3	2.08	0.53
1:B:132:GLY:C	1:B:134:ASP:N	2.63	0.53
1:A:160:GLN:O	1:A:168:ARG:NH2	2.41	0.53
1:A:78:LYS:O	1:A:79:HIS:HB2	2.09	0.53
1:B:336:LEU:HD22	1:B:340:GLN:CG	2.35	0.53
1:B:199:LYS:CA	1:B:237:TYR:HD1	2.18	0.52
1:B:236:PRO:HG2	1:B:237:TYR:HD2	1.65	0.52
1:A:226:ILE:C	1:A:226:ILE:HD12	2.29	0.52
1:A:205:SER:HB3	1:A:208:ARG:HB2	1.91	0.52
1:B:226:ILE:C	1:B:226:ILE:HD12	2.29	0.52
1:A:13:THR:HG21	1:A:89:GLU:OE1	2.10	0.52
1:B:314:LEU:HD11	1:B:349:MET:CG	2.30	0.52
1:B:336:LEU:HD13	1:B:340:GLN:NE2	2.25	0.52
1:A:259:PHE:O	1:A:261:PRO:HD2	2.10	0.52
1:A:267:LEU:O	1:A:270:LEU:HD12	2.09	0.52
1:B:41:LEU:HD22	1:B:144:TYR:HE1	1.75	0.52
1:A:226:ILE:HD11	1:A:249:PHE:CE2	2.44	0.52
1:B:170:LEU:HD11	1:B:238:ILE:HD11	1.91	0.52
1:B:89:GLU:O	1:B:90:ASN:HB2	2.10	0.52
1:B:41:LEU:HD22	1:B:144:TYR:CE1	2.45	0.52
1:B:275:ASP:C	1:B:277:VAL:H	2.13	0.51
1:A:156:GLY:O	1:A:157:HIS:HB2	2.10	0.51
1:A:273:VAL:CG1	1:A:274:GLN:N	2.73	0.51
1:A:198:ALA:C	1:A:200:GLY:N	2.62	0.51
1:B:201:LEU:O	1:B:203:GLY:N	2.44	0.51
1:B:336:LEU:HD22	1:B:340:GLN:NE2	2.26	0.51
1:A:60:MET:O	1:A:63:MET:HB3	2.11	0.51
1:A:115:TRP:C	1:A:117:LYS:H	2.13	0.51
1:A:210:TRP:CE3	1:A:210:TRP:HA	2.46	0.51
1:B:131:LEU:CD2	1:B:136:THR:O	2.49	0.51
1:B:198:ALA:C	1:B:200:GLY:N	2.61	0.51
1:B:201:LEU:O	1:B:204:ILE:HD12	2.11	0.51
1:A:209:ILE:HD12	1:A:238:ILE:HD12	1.93	0.51
1:B:278:THR:O	1:B:282:LEU:HG	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:TYR:CE2	1:B:200:GLY:HA3	2.46	0.51
1:A:35:GLY:O	1:A:36:ALA:HB2	2.10	0.50
1:B:318:GLN:O	1:B:322:ILE:HG13	2.11	0.50
1:B:245:SER:O	1:B:246:LEU:HB2	2.12	0.50
1:B:41:LEU:HD13	1:B:144:TYR:HD1	1.77	0.50
1:B:158:ALA:HB3	1:B:193:ALA:HB1	1.92	0.50
1:A:152:VAL:HG12	1:A:152:VAL:O	2.11	0.50
1:A:273:VAL:O	1:A:276:ASP:CB	2.59	0.50
1:A:344:CYS:SG	1:B:345:LEU:HD23	2.51	0.50
1:B:81:THR:HG23	1:B:94:THR:OG1	2.11	0.50
1:B:238:ILE:CG2	1:B:240:LEU:HG	2.42	0.50
1:B:85:ARG:NH2	1:B:88:GLU:HB3	2.27	0.50
1:A:115:TRP:C	1:A:117:LYS:N	2.65	0.50
1:B:158:ALA:C	1:B:160:GLN:N	2.65	0.50
1:B:146:ASP:C	1:B:147:LEU:O	2.47	0.50
1:A:330:THR:O	1:A:331:THR:C	2.50	0.49
1:A:79:HIS:O	1:A:81:THR:N	2.45	0.49
1:A:89:GLU:HB3	1:A:91:PHE:CE1	2.47	0.49
1:B:199:LYS:HB2	1:B:237:TYR:HE1	1.77	0.49
1:A:175:PHE:C	1:A:177:GLY:H	2.16	0.49
1:A:275:ASP:C	1:A:277:VAL:N	2.66	0.49
1:B:11:LEU:O	1:B:13:THR:N	2.43	0.49
1:A:210:TRP:CE2	1:A:286:ILE:HG22	2.48	0.49
1:A:38:ARG:HG2	1:A:38:ARG:HH21	1.78	0.49
1:B:229:ILE:HG22	1:B:229:ILE:O	2.12	0.49
1:A:175:PHE:C	1:A:177:GLY:N	2.65	0.49
1:B:3:LEU:C	1:B:3:LEU:HD23	2.32	0.49
1:B:71:MET:HA	1:B:83:THR:O	2.12	0.49
1:A:230:TYR:HE2	1:A:243:ASN:HA	1.78	0.49
1:A:5:SER:HB2	1:A:6:PRO:HD2	1.95	0.49
1:A:3:LEU:O	1:A:4:GLN:CG	2.60	0.49
1:B:201:LEU:O	1:B:204:ILE:CD1	2.60	0.49
1:A:210:TRP:HE3	1:A:210:TRP:HA	1.78	0.49
1:A:299:LYS:C	1:A:301:ARG:H	2.16	0.49
1:B:3:LEU:HD13	1:B:131:LEU:HD11	1.93	0.49
1:B:249:PHE:O	1:B:250:ASP:C	2.49	0.49
1:B:272:LYS:HZ1	1:B:302:LYS:CB	2.25	0.49
1:A:226:ILE:CG1	1:A:249:PHE:CZ	2.86	0.49
1:B:287:ALA:C	1:B:288:LYS:O	2.49	0.49
1:B:204:ILE:HD12	1:B:204:ILE:O	2.13	0.48
1:B:222:VAL:O	1:B:223:ASN:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:PHE:O	1:B:261:PRO:HD2	2.13	0.48
1:A:273:VAL:HG12	1:A:274:GLN:O	2.13	0.48
1:B:201:LEU:HD12	1:B:234:VAL:HG13	1.95	0.48
1:B:296:PHE:O	1:B:301:ARG:HG2	2.13	0.48
1:B:236:PRO:CG	1:B:237:TYR:CD2	2.89	0.48
1:B:56:THR:HB	1:B:57:PRO:HD2	1.95	0.48
1:A:281:ASP:HA	1:A:286:ILE:HG12	1.95	0.48
1:B:61:LYS:C	1:B:63:MET:N	2.65	0.48
1:A:176:TYR:CE1	1:A:186:HIS:CE1	3.02	0.48
1:B:11:LEU:O	1:B:16:LEU:HD12	2.13	0.48
1:B:224:HIS:O	1:B:227:HIS:N	2.45	0.48
1:A:137:LEU:C	1:A:137:LEU:HD13	2.34	0.48
1:B:36:ALA:HB1	1:B:49:ILE:HG23	1.95	0.48
1:A:297:ILE:O	1:A:302:LYS:HB2	2.14	0.48
1:B:209:ILE:HG13	1:B:210:TRP:N	2.28	0.48
1:A:156:GLY:O	1:A:157:HIS:CB	2.62	0.48
1:B:179:ILE:C	1:B:180:VAL:HG22	2.34	0.47
1:B:98:ILE:O	1:B:111:PHE:CD1	2.67	0.47
1:B:164:GLU:O	1:B:165:ASP:C	2.52	0.47
1:B:11:LEU:HD13	1:B:49:ILE:HD13	1.96	0.47
1:A:283:ARG:HG3	1:A:284:LEU:HD12	1.96	0.47
1:A:287:ALA:HB1	1:A:288:LYS:HG2	1.97	0.47
1:B:162:ILE:O	1:B:164:GLU:N	2.48	0.47
1:B:308:THR:HG22	1:B:309:ASP:N	2.29	0.47
1:A:96:LEU:N	1:A:96:LEU:HD12	2.30	0.47
1:B:224:HIS:O	1:B:225:LEU:C	2.53	0.47
1:B:230:TYR:CE1	1:B:235:ALA:HB2	2.50	0.47
1:B:23:PHE:CE2	1:B:30:LEU:HD12	2.49	0.47
1:A:19:LEU:HG	1:A:86:LEU:HD12	1.97	0.47
1:B:176:TYR:CD1	1:B:180:VAL:HG11	2.50	0.47
1:B:299:LYS:HA	1:B:302:LYS:HB3	1.97	0.47
1:A:95:THR:CG2	1:A:112:THR:HG23	2.43	0.47
1:A:147:LEU:O	1:A:149:ASN:N	2.46	0.47
1:B:211:VAL:HG12	1:B:211:VAL:O	2.13	0.47
1:A:235:ALA:N	1:A:236:PRO:HD2	2.31	0.46
1:B:162:ILE:HB	1:B:197:ASN:ND2	2.30	0.46
1:A:163:GLN:HG2	1:A:163:GLN:O	2.14	0.46
1:A:12:PHE:CD1	1:A:16:LEU:HD13	2.51	0.46
1:A:230:TYR:HE2	1:A:243:ASN:CA	2.29	0.46
1:B:165:ASP:C	1:B:167:LEU:N	2.66	0.46
1:A:205:SER:HB3	1:A:208:ARG:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:N	1:A:295:LEU:HD22	2.30	0.46
1:A:336:LEU:HD22	1:A:340:GLN:NE2	2.31	0.46
1:B:179:ILE:O	1:B:180:VAL:CG1	2.57	0.46
1:B:95:THR:HG21	1:B:112:THR:CG2	2.45	0.46
1:A:157:HIS:O	1:A:158:ALA:HB2	2.15	0.46
1:A:293:LEU:O	1:A:297:ILE:HG13	2.16	0.46
1:A:95:THR:HG22	1:A:96:LEU:N	2.31	0.46
1:B:94:THR:HG22	1:B:95:THR:O	2.16	0.46
1:B:205:SER:CB	1:B:208:ARG:HB2	2.46	0.46
1:A:139:ASP:O	1:A:140:TYR:CB	2.63	0.46
1:A:299:LYS:H	1:A:302:LYS:HB3	1.81	0.46
1:B:288:LYS:O	1:B:290:GLU:N	2.48	0.46
1:A:223:ASN:HA	1:A:249:PHE:HE2	1.81	0.46
1:B:335:GLU:OE1	1:B:338:LYS:HD2	2.15	0.46
1:A:166:TYR:CE2	1:A:200:GLY:HA3	2.50	0.46
1:B:335:GLU:OE1	1:B:338:LYS:CE	2.64	0.46
1:A:147:LEU:O	1:A:148:LYS:CB	2.57	0.46
1:B:31:ARG:NH2	1:B:116:GLN:NE2	2.63	0.46
1:B:175:PHE:O	1:B:177:GLY:N	2.49	0.46
1:A:28:HIS:CG	1:A:55:ALA:HB2	2.51	0.45
1:A:299:LYS:H	1:A:302:LYS:CB	2.29	0.45
1:A:180:VAL:O	1:A:181:ASP:HB2	2.15	0.45
1:A:222:VAL:O	1:A:223:ASN:C	2.54	0.45
1:A:238:ILE:O	1:A:238:ILE:HG23	2.16	0.45
1:A:275:ASP:H	1:A:277:VAL:HG12	1.81	0.45
1:A:313:PRO:O	1:A:314:LEU:HB3	2.15	0.45
1:A:160:GLN:C	1:A:163:GLN:HB3	2.37	0.45
1:A:179:ILE:HG13	1:A:179:ILE:O	2.15	0.45
1:B:313:PRO:O	1:B:314:LEU:CB	2.63	0.45
1:B:85:ARG:HE	1:B:90:ASN:ND2	2.14	0.45
1:A:315:LYS:N	1:A:316:PRO:CD	2.78	0.45
1:B:186:HIS:NE2	1:B:228:LEU:HD11	2.32	0.45
1:B:305:ILE:O	1:B:305:ILE:CG2	2.65	0.45
1:A:165:ASP:HB3	1:A:168:ARG:CD	2.46	0.45
1:A:201:LEU:O	1:A:204:ILE:HD12	2.17	0.45
1:A:207:GLU:O	1:A:211:VAL:HG23	2.15	0.45
1:A:214:LYS:O	1:A:218:VAL:HG23	2.17	0.45
1:A:308:THR:HG22	1:A:309:ASP:N	2.32	0.45
1:B:301:ARG:O	1:B:302:LYS:C	2.55	0.45
1:B:324:SER:O	1:B:325:ARG:C	2.54	0.45
1:A:96:LEU:HD23	1:A:118:ASP:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD23	1:A:4:GLN:HA	1.99	0.45
1:A:61:LYS:C	1:A:63:MET:N	2.71	0.45
1:A:13:THR:OG1	1:A:89:GLU:OE2	2.30	0.45
1:B:82:ILE:CG2	1:B:83:THR:N	2.80	0.45
1:A:201:LEU:O	1:A:204:ILE:CD1	2.66	0.45
1:B:156:GLY:O	1:B:157:HIS:O	2.34	0.45
1:A:194:ILE:O	1:A:195:ALA:C	2.54	0.44
1:B:175:PHE:O	1:B:176:TYR:C	2.55	0.44
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.57	0.44
1:A:56:THR:HB	1:A:57:PRO:HD2	1.99	0.44
1:B:14:GLU:HG2	1:B:14:GLU:H	1.49	0.44
1:B:165:ASP:HB3	1:B:168:ARG:NE	2.33	0.44
1:B:13:THR:HG21	1:B:89:GLU:OE1	2.16	0.44
1:A:259:PHE:O	1:A:261:PRO:CD	2.66	0.44
1:B:176:TYR:CE1	1:B:180:VAL:HG11	2.52	0.44
1:B:220:ASN:O	1:B:221:HIS:C	2.55	0.44
1:A:336:LEU:HD13	1:A:340:GLN:HE21	1.81	0.44
1:B:328:ASP:O	1:B:330:THR:N	2.50	0.44
1:A:235:ALA:O	1:A:238:ILE:HG22	2.18	0.44
1:A:243:ASN:HB2	1:A:244:ALA:H	1.28	0.44
1:B:123:ASP:O	1:B:155:VAL:HG22	2.18	0.44
1:B:124:LEU:O	1:B:125:THR:C	2.55	0.44
1:B:28:HIS:O	1:B:29:GLU:C	2.55	0.44
1:B:297:ILE:O	1:B:299:LYS:N	2.51	0.44
1:B:85:ARG:O	1:B:86:LEU:O	2.34	0.44
1:B:175:PHE:O	1:B:178:ARG:N	2.50	0.44
1:B:260:SER:N	1:B:338:LYS:HZ1	2.12	0.44
1:B:95:THR:CG2	1:B:112:THR:HG23	2.44	0.44
1:B:230:TYR:CE2	1:B:243:ASN:HA	2.53	0.44
1:B:335:GLU:O	1:B:338:LYS:HB2	2.17	0.44
1:A:301:ARG:O	1:A:302:LYS:C	2.57	0.43
1:B:300:ASN:C	1:B:301:ARG:HD3	2.39	0.43
1:B:78:LYS:O	1:B:79:HIS:C	2.56	0.43
1:A:180:VAL:HG23	1:A:181:ASP:H	1.82	0.43
1:A:336:LEU:HD22	1:A:340:GLN:HE21	1.82	0.43
1:B:328:ASP:O	1:B:331:THR:N	2.51	0.43
1:B:95:THR:HG22	1:B:96:LEU:N	2.33	0.43
1:B:137:LEU:O	1:B:138:PHE:CB	2.66	0.43
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.18	0.43
1:A:20:THR:O	1:A:21:GLU:C	2.54	0.43
1:A:19:LEU:CD1	1:A:91:PHE:CD2	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:C	1:B:203:GLY:H	2.22	0.43
1:B:270:LEU:HD23	1:B:270:LEU:H	1.84	0.43
1:B:295:LEU:HA	1:B:298:VAL:HB	2.00	0.43
1:A:61:LYS:O	1:A:65:GLN:HB2	2.19	0.43
1:B:190:THR:O	1:B:194:ILE:HG13	2.19	0.43
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.90	0.43
1:A:159:LYS:N	1:A:159:LYS:HD2	2.33	0.43
1:A:176:TYR:CD1	1:A:186:HIS:CE1	3.06	0.43
1:A:209:ILE:HD12	1:A:238:ILE:HG13	1.99	0.43
1:A:3:LEU:O	1:A:4:GLN:HG3	2.19	0.43
1:A:299:LYS:HG2	1:A:302:LYS:HD2	2.00	0.43
1:B:96:LEU:HD21	1:B:116:GLN:OE1	2.18	0.43
1:A:328:ASP:O	1:A:330:THR:N	2.52	0.43
1:A:6:PRO:HG2	1:A:7:GLU:H	1.84	0.43
1:B:271:PHE:CE1	1:B:277:VAL:HA	2.54	0.43
1:B:7:GLU:O	1:B:10:SER:OG	2.35	0.43
1:A:288:LYS:H	1:A:288:LYS:HD3	1.84	0.42
1:A:53:THR:O	1:A:95:THR:HA	2.19	0.42
1:B:31:ARG:HH21	1:B:116:GLN:HE22	1.66	0.42
1:B:151:LYS:O	1:B:152:VAL:CB	2.59	0.42
1:B:229:ILE:CG2	1:B:229:ILE:O	2.67	0.42
1:B:5:SER:HB2	1:B:6:PRO:HD2	2.00	0.42
1:A:169:ILE:CD1	1:A:198:ALA:HA	2.49	0.42
1:A:288:LYS:H	1:A:288:LYS:CD	2.27	0.42
1:A:288:LYS:C	1:A:290:GLU:N	2.73	0.42
1:A:326:GLU:HA	1:A:327:PRO:HD3	1.85	0.42
1:B:175:PHE:C	1:B:177:GLY:H	2.22	0.42
1:B:44:VAL:HG23	1:B:44:VAL:O	2.19	0.42
1:A:198:ALA:C	1:A:200:GLY:H	2.21	0.42
1:A:201:LEU:O	1:A:203:GLY:N	2.52	0.42
1:A:202:ALA:HB2	1:A:237:TYR:HD1	1.84	0.42
1:A:295:LEU:HD13	1:A:295:LEU:H	1.84	0.42
1:B:147:LEU:O	1:B:149:ASN:N	2.46	0.42
1:B:169:ILE:CD1	1:B:198:ALA:HA	2.49	0.42
1:A:249:PHE:O	1:A:250:ASP:C	2.58	0.42
1:B:147:LEU:O	1:B:148:LYS:HB3	2.19	0.42
1:B:201:LEU:C	1:B:203:GLY:N	2.71	0.42
1:B:276:ASP:C	1:B:276:ASP:OD2	2.58	0.42
1:A:204:ILE:O	1:A:205:SER:C	2.58	0.42
1:B:225:LEU:O	1:B:229:ILE:HG13	2.19	0.42
1:A:41:LEU:HD22	1:A:144:TYR:HE1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:HIS:HE1	1:B:250:ASP:OD2	2.03	0.42
1:B:160:GLN:CA	1:B:163:GLN:HB3	2.47	0.42
1:B:204:ILE:O	1:B:205:SER:C	2.58	0.42
1:B:61:LYS:O	1:B:63:MET:N	2.52	0.42
1:A:83:THR:HA	1:A:91:PHE:O	2.20	0.42
1:B:171:ARG:O	1:B:175:PHE:HD1	2.03	0.42
1:B:176:TYR:O	1:B:180:VAL:HG21	2.20	0.42
1:B:36:ALA:CB	1:B:49:ILE:HG23	2.49	0.42
1:B:11:LEU:HD21	1:B:46:PRO:CG	2.49	0.42
1:B:176:TYR:O	1:B:180:VAL:CG2	2.68	0.42
1:B:230:TYR:CD1	1:B:235:ALA:HB2	2.54	0.41
1:B:277:VAL:O	1:B:280:LEU:HB3	2.20	0.41
1:A:117:LYS:HZ2	1:A:140:TYR:HD2	1.61	0.41
1:A:318:GLN:O	1:A:319:ASP:C	2.57	0.41
1:A:39:ASP:O	1:A:42:ASN:N	2.53	0.41
1:A:72:ILE:CD1	1:A:90:ASN:ND2	2.82	0.41
1:B:138:PHE:N	1:B:138:PHE:CD2	2.87	0.41
1:B:230:TYR:HE2	1:B:243:ASN:HA	1.84	0.41
1:B:259:PHE:H	1:B:259:PHE:HD1	1.66	0.41
1:B:267:LEU:O	1:B:268:ALA:C	2.56	0.41
1:B:238:ILE:HG23	1:B:238:ILE:O	2.20	0.41
1:B:85:ARG:CD	1:B:88:GLU:HA	2.50	0.41
1:B:298:VAL:C	1:B:300:ASN:H	2.16	0.41
1:A:313:PRO:O	1:A:314:LEU:CB	2.69	0.41
1:B:248:GLU:O	1:B:251:LYS:HB2	2.21	0.41
1:B:297:ILE:O	1:B:298:VAL:C	2.59	0.41
1:B:315:LYS:HA	1:B:318:GLN:HE21	1.85	0.41
1:B:38:ARG:NH2	1:B:38:ARG:HG2	2.34	0.41
1:A:147:LEU:HG	1:A:148:LYS:N	2.35	0.41
1:A:228:LEU:HD22	1:A:232:LEU:CD1	2.51	0.41
1:B:147:LEU:C	1:B:149:ASN:N	2.72	0.41
1:A:30:LEU:CD2	1:A:30:LEU:C	2.88	0.41
1:A:33:ALA:HA	1:A:37:VAL:CG2	2.51	0.41
1:A:260:SER:H	1:A:338:LYS:HZ1	1.69	0.40
1:A:38:ARG:O	1:A:39:ASP:C	2.59	0.40
1:B:39:ASP:O	1:B:42:ASN:N	2.54	0.40
1:B:46:PRO:O	1:B:47:GLN:CB	2.68	0.40
1:A:275:ASP:N	1:A:277:VAL:HG12	2.36	0.40
1:A:277:VAL:O	1:A:280:LEU:HB3	2.21	0.40
1:A:314:LEU:HD11	1:A:349:MET:CG	2.48	0.40
1:A:19:LEU:HD11	1:A:93:ILE:HD11	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:THR:O	1:A:332:ARG:C	2.59	0.40
1:A:71:MET:HA	1:A:83:THR:O	2.20	0.40
1:A:85:ARG:HG2	1:A:90:ASN:HD21	1.86	0.40
1:B:248:GLU:O	1:B:249:PHE:C	2.60	0.40
1:B:262:LYS:O	1:B:263:PRO:C	2.60	0.40
1:B:252:VAL:HG11	1:B:339:TYR:CD2	2.56	0.40
1:B:54:THR:HA	1:B:96:LEU:CD1	2.52	0.40
1:A:342:GLU:HB3	1:A:345:LEU:HD12	2.04	0.40
1:B:111:PHE:O	1:B:112:THR:C	2.60	0.40
1:B:155:VAL:HG23	1:B:155:VAL:O	2.22	0.40
1:B:180:VAL:HG23	1:B:181:ASP:H	1.87	0.40
1:A:205:SER:CB	1:A:208:ARG:HB2	2.51	0.40
1:A:228:LEU:HD22	1:A:232:LEU:HD11	2.04	0.40
1:A:38:ARG:HG2	1:A:38:ARG:NH2	2.37	0.40
1:B:205:SER:HB3	1:B:208:ARG:HB2	2.02	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:18:SER:OG	1:B:328:ASP:OD2[4_565]	2.17	0.03

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	342/448 (76%)	229 (67%)	78 (23%)	35 (10%)	0 4
1	B	342/448 (76%)	227 (66%)	75 (22%)	40 (12%)	0 3
All	All	684/896 (76%)	456 (67%)	153 (22%)	75 (11%)	0 3

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	79	HIS
1	A	80	GLY
1	A	86	LEU
1	A	112	THR
1	A	116	GLN
1	A	158	ALA
1	A	165	ASP
1	A	243	ASN
1	A	244	ALA
1	A	245	SER
1	A	298	VAL
1	B	79	HIS
1	B	86	LEU
1	B	112	THR
1	B	157	HIS
1	B	165	ASP
1	B	180	VAL
1	B	205	SER
1	B	221	HIS
1	B	243	ASN
1	B	298	VAL
1	A	36	ALA
1	A	123	ASP
1	A	157	HIS
1	A	163	GLN
1	A	180	VAL
1	A	183	PRO
1	A	205	SER
1	B	74	ASN
1	B	158	ALA
1	B	163	GLN
1	B	275	ASP
1	B	294	GLY
1	A	47	GLN
1	A	75	ARG
1	A	181	ASP
1	A	185	ASP
1	A	306	LYS
1	B	27	ASN
1	B	181	ASP
1	B	202	ALA
1	B	299	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	328	ASP
1	A	88	GLU
1	A	202	ALA
1	A	308	THR
1	B	47	GLN
1	B	62	GLU
1	B	90	ASN
1	B	116	GLN
1	B	302	LYS
1	B	308	THR
1	B	329	ALA
1	A	27	ASN
1	A	90	ASN
1	A	152	VAL
1	A	241	PRO
1	A	299	LYS
1	B	88	GLU
1	B	98	ILE
1	B	138	PHE
1	B	140	TYR
1	B	198	ALA
1	B	249	PHE
1	B	300	ASN
1	A	98	ILE
1	A	249	PHE
1	B	224	HIS
1	B	225	LEU
1	B	233	ASP
1	B	244	ALA
1	B	152	VAL
1	B	312	ASP
1	A	294	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	304/393 (77%)	270 (89%)	34 (11%)	6 22
1	B	304/393 (77%)	271 (89%)	33 (11%)	6 23
All	All	608/786 (77%)	541 (89%)	67 (11%)	6 23

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	14	GLU
1	A	16	LEU
1	A	17	LYS
1	A	19	LEU
1	A	29	GLU
1	A	32	ILE
1	A	38	ARG
1	A	48	ASP
1	A	85	ARG
1	A	115	TRP
1	A	134	ASP
1	A	142	ASN
1	A	160	GLN
1	A	161	ARG
1	A	162	ILE
1	A	168	ARG
1	A	178	ARG
1	A	180	VAL
1	A	183	PRO
1	A	199	LYS
1	A	207	GLU
1	A	210	TRP
1	A	221	HIS
1	A	243	ASN
1	A	270	LEU
1	A	272	LYS
1	A	275	ASP
1	A	288	LYS
1	A	292	ASN
1	A	295	LEU
1	A	326	GLU
1	A	336	LEU
1	A	349	MET
1	B	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	7	GLU
1	B	9	GLN
1	B	14	GLU
1	B	16	LEU
1	B	17	LYS
1	B	19	LEU
1	B	29	GLU
1	B	32	ILE
1	B	38	ARG
1	B	48	ASP
1	B	85	ARG
1	B	115	TRP
1	B	121	ARG
1	B	134	ASP
1	B	137	LEU
1	B	138	PHE
1	B	142	ASN
1	B	157	HIS
1	B	161	ARG
1	B	165	ASP
1	B	168	ARG
1	B	171	ARG
1	B	180	VAL
1	B	199	LYS
1	B	207	GLU
1	B	221	HIS
1	B	237	TYR
1	B	272	LYS
1	B	295	LEU
1	B	323	ASP
1	B	336	LEU
1	B	349	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	160	GLN
1	A	227	HIS
1	A	255	ASN
1	A	318	GLN
1	A	340	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4	GLN
1	B	9	GLN
1	B	28	HIS
1	B	42	ASN
1	B	65	GLN
1	B	73	ASN
1	B	90	ASN
1	B	142	ASN
1	B	160	GLN
1	B	163	GLN
1	B	227	HIS
1	B	255	ASN
1	B	292	ASN
1	B	318	GLN
1	B	340	GLN
1	B	343	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	340/448 (75%)	0.10	5 (1%)	73	72	26, 26, 26, 26	56 (16%)
1	B	344/448 (76%)	0.08	4 (1%)	79	77	26, 26, 26, 26	47 (13%)
All	All	684/896 (76%)	0.09	9 (1%)	77	76	26, 26, 26, 26	103 (15%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	THR	4.1
1	A	188	PRO	3.1
1	A	84	ALA	3.0
1	B	321	ILE	3.0
1	B	30	LEU	2.6
1	A	52	ALA	2.5
1	B	96	LEU	2.4
1	B	79	HIS	2.4
1	A	30	LEU	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.