



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:24 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

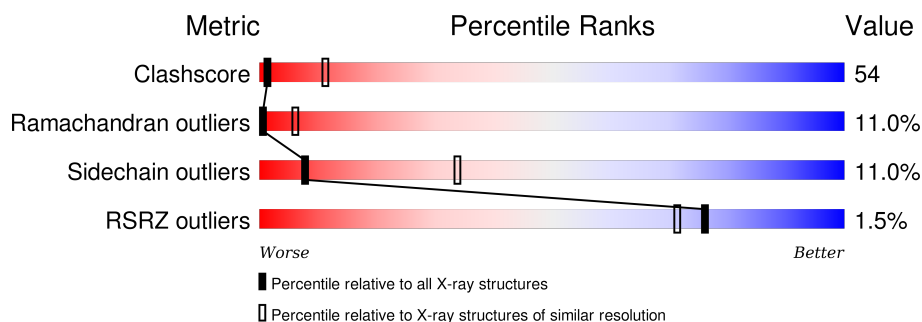
1 Overall quality at a glance

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	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (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. 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	448	
1	B	448	

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

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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

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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

Lys	K299	D233	K159
	GLU	V234	K160
	ILE	A235	K161
	GLY	P236	I162
	ALA	Y237	Q163
	LEU	I238	E164
	LEU	G239	D165
	GLN	L240	K166
	GLN	P241	K167
	LEU	A242	K168
Arg	S311	D243	I169
	GLU	A244	L170
	GLN	S245	K171
	TRP	L246	
	Lys	E247	F175
	Lys	E248	Y176
	Lys	F249	G177
	Ser	D250	R178
	GLY	K251	I179
	TYR	V252	R180
Gln	I321		D181
	I322	V256	H186
	GLU	D257	D187
	MET	G258	
	GLU	F259	T190
	GLU	S260	
	LEU	P261	A193
	LEU	K262	I194
	LEU	F271	
	TYR	K272	N197
Lys	Q340	V273	A198
		Q274	K199
	I345	D275	G200
	K349	D276	L201
		V277	A202
	I354	T278	G203
	PRO	K279	S205
	PRO	L280	G206
	PRO	D281	E207
	VAL	L282	K208
Ser	GLY	R283	I209
	GLY	L284	W210
	His	A287	V211
	ASP	K288	
	ILE	E289	I216
	ARG	E290	N220
	Lys		H221
	VAL	L293	N223
	GLY	G294	H224
	ILE	L295	L225
Lys	Ser	F296	I226
	Ser	T297	L227
	GLY	V298	L228
			L229
			Y230

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.278 , 0.318 0.296 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20358 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 ⓘ

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:B:272:LYS:HE2	1:B:299:LYS:H	1.35	0.90
1:A:209:ILE:HD11	1:A:284:LEU:HD11	1.52	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

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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:B:46:PRO:HB2	1:B:49:ILE:HG12	1.64	0.79
1:A:39:ASP:HB3	1:A:44:VAL:HG23	1.65	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:B:11:LEU:HD22	1:B:49:ILE:HD11	1.72	0.71
1:A:287:ALA:O	1:A:290:GLU:HB2	1.89	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

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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: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:288:LYS:O	1:A:290:GLU:N	2.24	0.67
1:A:230:TYR:HD2	1:A:243:ASN:HB3	1.53	0.67
1:B:237:TYR:HD2	1:B:237:TYR:H	1.39	0.67
1:A:178:ARG:HH21	1:A:178:ARG:HG3	1.60	0.67
1:A:210:TRP:CE3	1:A:284:LEU:HD23	2.29	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:315:LYS:N	1:A:316:PRO:HD2	2.10	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:305:ILE:O	1:B:305:ILE:HG23	1.94	0.66
1:B:130:PHE:O	1:B:137:LEU:O	2.14	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:B:301:ARG:O	1:B:305:ILE:HG22	1.96	0.65
1:A:273:VAL:O	1:A:276:ASP:HB3	1.97	0.65
1:A:139:ASP:O	1:A:140:TYR:HB2	1.97	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:B:31:ARG:HD3	1:B:116:GLN:HE22	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TRP:O	1:A:117:LYS:N	2.30	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:B:180:VAL:O	1:B:181:ASP:CB	2.45	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: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:B:280:LEU:CD1	1:B:284:LEU:HD22	2.30	0.62
1:A:308:THR:O	1:A:309:ASP:HB2	1.99	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:B:201:LEU:HD13	1:B:238:ILE:HD13	1.82	0.61
1:A:158:ALA:C	1:A:160:GLN:H	2.01	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:280:LEU:CD1	1:A:284:LEU:HD22	2.30	0.60
1:A:23:PHE:CD2	1:A:30:LEU:HD12	2.37	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

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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: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:292:ASN:HA	1:A:295:LEU:HD21	1.84	0.60
1:B:236:PRO:CG	1:B:237:TYR:CE2	2.85	0.59
1:A:328:ASP:O	1:A:329:ALA:C	2.40	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:A:11:LEU:HD21	1:A:46:PRO:HG2	1.84	0.59
1:B:308:THR:O	1:B:309:ASP:OD1	2.18	0.59
1:A:30:LEU:C	1:A:30:LEU:HD23	2.23	0.59
1:A:179:ILE:O	1:A:180:VAL:HG13	2.02	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:275:ASP:C	1:A:277:VAL:H	2.05	0.58
1:A:41:LEU:HD13	1:A:144:TYR:CD1	2.37	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:B:283:ARG:HG3	1:B:284:LEU:HD12	1.85	0.57
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:209:ILE:HD11	1:B:284:LEU:CD1	2.22	0.57
1:B:31:ARG:NH2	1:B:116:GLN:HE22	2.02	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:B:235:ALA:N	1:B:236:PRO:HD2	2.19	0.57
1:A:11:LEU:HD21	1:A:46:PRO:CG	2.34	0.57
1:B:335:GLU:OE1	1:B:338:LYS:HE3	2.05	0.57
1:B:289:GLU:O	1:B:293:LEU:N	2.34	0.57
1:B:199:LYS:HA	1:B:237:TYR:HD1	1.58	0.57
1:A:315:LYS:HA	1:A:318:GLN:HE21	1.70	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

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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:61:LYS:C	1:A:63:MET:H	2.07	0.56
1:A:186:HIS:HB3	1:A:191:LEU:HD13	1.87	0.56
1:B:313:PRO:O	1:B:314:LEU:HB3	2.05	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:242:ALA:O	1:B:243:ASN:C	2.42	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: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:B:98:ILE:O	1:B:111:PHE:HD1	1.90	0.55
1:A:199:LYS:HA	1:A:237:TYR:CE1	2.42	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:283:ARG:HG3	1:A:284:LEU:CD1	2.37	0.55
1:A:147:LEU:C	1:A:149:ASN:N	2.60	0.55
1:B:274:GLN:HG3	1:B:295:LEU:HB3	1.90	0.54
1:B:146:ASP:CB	1:B:151:LYS:HB3	2.33	0.54
1:B:223:ASN:HA	1:B:249:PHE:HE2	1.71	0.54
1:A:160:GLN:HA	1:A:163:GLN:HB2	1.89	0.54
1:B:315:LYS:N	1:B:316:PRO:CD	2.70	0.54
1:B:241:PRO:HG3	1:B:271:PHE:CB	2.22	0.54
1:B:160:GLN:HA	1:B:163:GLN:CB	2.37	0.54
1:A:81:THR:HG23	1:A:94:THR:OG1	2.07	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:299:LYS:C	1:B:301:ARG:N	2.61	0.53
1:B:163:GLN:O	1:B:163:GLN:HG2	2.08	0.53
1:B:336:LEU:HD22	1:B:340:GLN:HE21	1.74	0.53
1:B:119:ALA:O	1:B:141:PHE:CZ	2.62	0.53
1:A:164:GLU:O	1:A:165:ASP:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:HB	1:A:261:PRO:HB3	1.91	0.53
1:A:180:VAL:O	1:A:181:ASP:CB	2.56	0.53
1:A:84:ALA:O	1:A:90:ASN:HA	2.08	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:250:ASP:O	1:A:253:SER:HB3	2.08	0.53
1:A:165:ASP:HB3	1:A:168:ARG:HD3	1.90	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:B:336:LEU:HD22	1:B:340:GLN:CG	2.35	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: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: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:13:THR:HG21	1:A:89:GLU:OE1	2.10	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:273:VAL:CG1	1:A:274:GLN:N	2.73	0.51
1:A:156:GLY:O	1:A:157:HIS:HB2	2.10	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:198:ALA:C	1:A:200:GLY:N	2.62	0.51
1:A:60:MET:O	1:A:63:MET:HB3	2.11	0.51
1:B:131:LEU:CD2	1:B:136:THR:O	2.49	0.51
1:A:210:TRP:CE3	1:A:210:TRP:HA	2.46	0.51
1:B:198:ALA:C	1:B:200:GLY:N	2.61	0.51
1:A:115:TRP:C	1:A:117:LYS:H	2.13	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

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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:158:ALA:HB3	1:B:193:ALA:HB1	1.92	0.50
1:B:41:LEU:HD13	1:B:144:TYR:HD1	1.77	0.50
1:A:273:VAL:O	1:A:276:ASP:CB	2.59	0.50
1:A:152:VAL:HG12	1:A:152:VAL:O	2.11	0.50
1:B:81:THR:HG23	1:B:94:THR:OG1	2.11	0.50
1:A:344:CYS:SG	1:B:345:LEU:HD23	2.51	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:B:199:LYS:HB2	1:B:237:TYR:HE1	1.77	0.49
1:A:89:GLU:HB3	1:A:91:PHE:CE1	2.47	0.49
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: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:175:PHE:C	1:A:177:GLY:H	2.16	0.49
1:A:210:TRP:CE2	1:A:286:ILE:HG22	2.48	0.49
1:B:229:ILE:HG22	1:B:229:ILE:O	2.12	0.49
1:A:38:ARG:HG2	1:A:38:ARG:HH21	1.78	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:175:PHE:C	1:A:177:GLY:N	2.65	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:B:201:LEU:O	1:B:204:ILE:CD1	2.60	0.49
1:A:3:LEU:O	1:A:4:GLN:CG	2.60	0.49
1:A:210:TRP:HE3	1:A:210:TRP:HA	1.78	0.49
1:B:272:LYS:HZ1	1:B:302:LYS:CB	2.25	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:A:299:LYS:C	1:A:301:ARG:H	2.16	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:O	1:B:204:ILE:HD12	2.13	0.48
1:B:222:VAL:O	1:B:223:ASN:C	2.51	0.48

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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: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:A:273:VAL:HG12	1:A:274:GLN:O	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:B:11:LEU:O	1:B:16:LEU:HD12	2.13	0.48
1:A:176:TYR:CE1	1:A:186:HIS:CE1	3.02	0.48
1:B:224:HIS:O	1:B:227:HIS:N	2.45	0.48
1:B:36:ALA:HB1	1:B:49:ILE:HG23	1.95	0.48
1:A:137:LEU:C	1:A:137:LEU:HD13	2.34	0.48
1:B:209:ILE:HG13	1:B:210:TRP:N	2.28	0.48
1:A:297:ILE:O	1:A:302:LYS:HB2	2.14	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:164:GLU:O	1:B:165:ASP:C	2.52	0.47
1:B:98:ILE:O	1:B:111:PHE:CD1	2.67	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:B:162:ILE:O	1:B:164:GLU:N	2.48	0.47
1:A:287:ALA:HB1	1:A:288:LYS:HG2	1.97	0.47
1:B:230:TYR:CE1	1:B:235:ALA:HB2	2.50	0.47
1:B:308:THR:HG22	1:B:309:ASP:N	2.29	0.47
1:B:224:HIS:O	1:B:225:LEU:C	2.53	0.47
1:A:96:LEU:N	1:A:96:LEU:HD12	2.30	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:299:LYS:HA	1:B:302:LYS:HB3	1.97	0.47
1:B:176:TYR:CD1	1:B:180:VAL:HG11	2.50	0.47
1:A:147:LEU:O	1:A:149:ASN:N	2.46	0.47
1:A:95:THR:CG2	1:A:112:THR:HG23	2.43	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: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:12:PHE:CD1	1:A:16:LEU:HD13	2.51	0.46
1:A:163:GLN:HG2	1:A:163:GLN:O	2.14	0.46
1:A:205:SER:HB3	1:A:208:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HD22	1:A:295:LEU:N	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:293:LEU:O	1:A:297:ILE:HG13	2.16	0.46
1:A:157:HIS:O	1:A:158:ALA:HB2	2.15	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:299:LYS:H	1:A:302:LYS:HB3	1.81	0.46
1:A:139:ASP:O	1:A:140:TYR:CB	2.63	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:B:175:PHE:O	1:B:177:GLY:N	2.49	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:A:299:LYS:H	1:A:302:LYS:CB	2.29	0.45
1:A:28:HIS:CG	1:A:55:ALA:HB2	2.51	0.45
1:A:222:VAL:O	1:A:223:ASN:C	2.54	0.45
1:A:180:VAL:O	1:A:181:ASP:HB2	2.15	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: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: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:305:ILE:O	1:B:305:ILE:CG2	2.65	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:301:ARG:O	1:B:302:LYS:C	2.55	0.45
1:A:308:THR:HG22	1:A:309:ASP:N	2.32	0.45
1:A:201:LEU:O	1:A:204:ILE:HD12	2.17	0.45
1:A:165:ASP:HB3	1:A:168:ARG:CD	2.46	0.45
1:A:207:GLU:O	1:A:211:VAL:HG23	2.15	0.45
1:B:324:SER:O	1:B:325:ARG:C	2.54	0.45
1:A:214:LYS:O	1:A:218:VAL:HG23	2.17	0.45
1:A:61:LYS:C	1:A:63:MET:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:OG1	1:A:89:GLU:OE2	2.30	0.45
1:A:96:LEU:HD23	1:A:118:ASP:HB2	1.98	0.45
1:B:82:ILE:CG2	1:B:83:THR:N	2.80	0.45
1:A:3:LEU:HD23	1:A:4:GLN:HA	1.99	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:B:175:PHE:O	1:B:176:TYR:C	2.55	0.44
1:A:194:ILE:O	1:A:195:ALA:C	2.54	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:56:THR:HB	1:A:57:PRO:HD2	1.99	0.44
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.57	0.44
1:B:14:GLU:HG2	1:B:14:GLU:H	1.49	0.44
1:B:176:TYR:CE1	1:B:180:VAL:HG11	2.52	0.44
1:A:259:PHE:O	1:A:261:PRO:CD	2.66	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:B:297:ILE:O	1:B:299:LYS:N	2.51	0.44
1:A:243:ASN:HB2	1:A:244:ALA:H	1.28	0.44
1:A:235:ALA:O	1:A:238:ILE:HG22	2.18	0.44
1:B:85:ARG:O	1:B:86:LEU:O	2.34	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:123:ASP:O	1:B:155:VAL:HG22	2.18	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: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:B:95:THR:CG2	1:B:112:THR:HG23	2.44	0.44
1:B:300:ASN:C	1:B:301:ARG:HD3	2.39	0.43
1:A:301:ARG:O	1:A:302:LYS:C	2.57	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:95:THR:HG22	1:B:96:LEU:N	2.33	0.43
1:B:328:ASP:O	1:B:331:THR:N	2.51	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:B:201:LEU:C	1:B:203:GLY:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HA	1:B:298:VAL:HB	2.00	0.43
1:B:270:LEU:HD23	1:B:270:LEU:H	1.84	0.43
1:A:19:LEU:CD1	1:A:91:PHE:CD2	2.97	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:209:ILE:HD12	1:A:238:ILE:HG13	1.99	0.43
1:A:176:TYR:CD1	1:A:186:HIS:CE1	3.06	0.43
1:A:3:LEU:O	1:A:4:GLN:HG3	2.19	0.43
1:A:159:LYS:N	1:A:159:LYS:HD2	2.33	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:B:271:PHE:CE1	1:B:277:VAL:HA	2.54	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:7:GLU:O	1:B:10:SER:OG	2.35	0.43
1:B:229:ILE:O	1:B:229:ILE:CG2	2.67	0.42
1:B:151:LYS:O	1:B:152:VAL:CB	2.59	0.42
1:A:288:LYS:HD3	1:A:288:LYS:H	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:5:SER:HB2	1:B:6:PRO:HD2	2.00	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:169:ILE:CD1	1:A:198:ALA:HA	2.49	0.42
1:A:288:LYS:CD	1:A:288:LYS:H	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:A:201:LEU:O	1:A:203:GLY:N	2.52	0.42
1:A:198:ALA:C	1:A:200:GLY:H	2.21	0.42
1:A:202:ALA:HB2	1:A:237:TYR:HD1	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:295:LEU:HD13	1:A:295:LEU:H	1.84	0.42
1:B:201:LEU:C	1:B:203:GLY:N	2.71	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:276:ASP:OD2	1:B:276:ASP:C	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:B:227:HIS:HE1	1:B:250:ASP:OD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD22	1:A:144:TYR:HE1	1.85	0.42
1:B:204:ILE:O	1:B:205:SER:C	2.58	0.42
1:B:160:GLN:CA	1:B:163:GLN:HB3	2.47	0.42
1:B:61:LYS:O	1:B:63:MET:N	2.52	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:A:83:THR:HA	1:A:91:PHE:O	2.20	0.42
1:B:176:TYR:O	1:B:180:VAL:CG2	2.68	0.42
1:B:11:LEU:HD21	1:B:46:PRO:CG	2.49	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:B:230:TYR:HE2	1:B:243:ASN:HA	1.84	0.41
1:B:267:LEU:O	1:B:268:ALA:C	2.56	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:A:318:GLN:O	1:A:319:ASP:C	2.57	0.41
1:B:138:PHE:N	1:B:138:PHE:CD2	2.87	0.41
1:A:117:LYS:HZ2	1:A:140:TYR:HD2	1.61	0.41
1:B:259:PHE:H	1:B:259:PHE:HD1	1.66	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:B:297:ILE:O	1:B:298:VAL:C	2.59	0.41
1:B:248:GLU:O	1:B:251:LYS:HB2	2.21	0.41
1:A:313:PRO:O	1:A:314:LEU:CB	2.69	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:B:147:LEU:C	1:B:149:ASN:N	2.72	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: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: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:38:ARG:O	1:A:39:ASP:C	2.59	0.40
1:A:260:SER:H	1:A:338:LYS:HZ1	1.69	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:19:LEU:HD11	1:A:93:ILE:HD11	2.02	0.40
1:A:314:LEU:HD11	1:A:349:MET:CG	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:O	1:B:249:PHE:C	2.60	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:54:THR:HA	1:B:96:LEU:CD1	2.52	0.40
1:A:331:THR:O	1:A:332:ARG:C	2.59	0.40
1:B:252:VAL:HG11	1:B:339:TYR:CD2	2.56	0.40
1:B:262:LYS:O	1:B:263:PRO:C	2.60	0.40
1:B:180:VAL:HG23	1:B:181:ASP:H	1.87	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:A:342:GLU:HB3	1:A:345:LEU:HD12	2.04	0.40
1:B:205:SER:HB3	1:B:208:ARG:HB2	2.02	0.40
1:A:205:SER:CB	1:A:208:ARG:HB2	2.51	0.40
1:A:38:ARG:NH2	1:A:38:ARG:HG2	2.37	0.40
1:A:228:LEU:HD22	1:A:232:LEU:HD11	2.04	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%)	1	7
1	B	342/448 (76%)	227 (66%)	75 (22%)	40 (12%)	0	5
All	All	684/896 (76%)	456 (67%)	153 (22%)	75 (11%)	0	6

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

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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 ⓘ

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%)	7	32
1	B	304/393 (77%)	271 (89%)	33 (11%)	8	34
All	All	608/786 (77%)	541 (89%)	67 (11%)	8	34

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

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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

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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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	340/448 (75%)	0.12	5 (1%) 76 71	26, 26, 26, 26	56 (16%)
1	B	344/448 (76%)	0.11	5 (1%) 76 71	26, 26, 26, 26	47 (13%)
All	All	684/896 (76%)	0.12	10 (1%) 76 71	26, 26, 26, 26	103 (15%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	THR	4.3
1	A	188	PRO	3.2
1	A	84	ALA	3.1
1	B	321	ILE	3.1
1	B	30	LEU	2.6
1	A	52	ALA	2.5
1	B	96	LEU	2.5
1	B	79	HIS	2.5
1	A	30	LEU	2.2
1	B	81	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.