



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:45 am BST

PDB ID : 3T53
Title : Crystal structures of the extrusion state of the CusBA adaptor-transporter complex
Authors : Su, C.-C.; Long, F.; Yu, E.W.
Deposited on : 2011-07-26
Resolution : 3.37 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

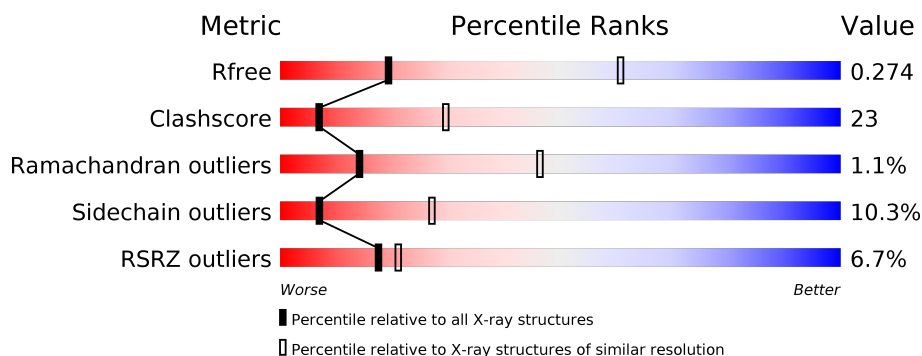
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 $\leq 5\%$. 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	B	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 36%, green 56%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 56% 36% • • </div> </div>
1	C	336	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 35%, green 57%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 57% 35% • • </div> </div>
2	A	1054	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 41%, green 51%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 10% 51% 41% 5% • </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12876 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 Cation efflux system protein CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1028	Total	C	N	O	S	0	0	0
			7923	5124	1330	1433	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0


- Molecule 4 is water.

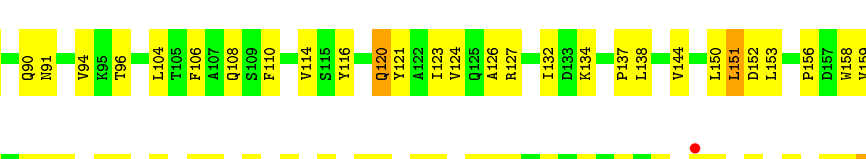
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total O 4 4	0	0
4	C	10	Total O 10 10	0	0
4	A	7	Total O 7 7	0	0

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.

- Chain B:

Category	Percentage	Amino Acids
Green	56%	L371, L372, E375, K376, V377, V378, F383, L384, I385, D386, E387, E388, A389, K390, I391, A394, L395, E396, R399, S400, SER, GLU, ALA, THR, HIS, HIS, HIS, HIS, HIS, HIS, HIS, HIS
Yellow	36%	K280, W281, T282, V287, T291, R292, T293, L294, R297, L298, N302, A306, L307, K308, P309, E322, P323, M324, I327, Q330, A331, L332, T335, G336, S337, E338, Q339, V341, I342, T343, V344, G348, R349, F350, V351, R354, V355, A356, V357, F358, Q359, A360, S361, V364, T365, P368
Orange		K280, W281, T282, V287, T291, R292, T293, L294, R297, L298, N302, A306, L307, K308, P309, E322, P323, M324, I327, Q330, A331, L332, T335, G336, S337, E338, Q339, V341, I342, T343, V344, G348, R349, F350, V351, R354, V355, A356, V357, F358, Q359, A360, S361, V364, T365, P368
Red		K280, W281, T282, V287, T291, R292, T293, L294, R297, L298, N302, A306, L307, K308, P309, E322, P323, M324, I327, Q330, A331, L332, T335, G336, S337, E338, Q339, V341, I342, T343, V344, G348, R349, F350, V351, R354, V355, A356, V357, F358, Q359, A360, S361, V364, T365, P368

- Chain C: 



Item	SER	Item	SER	Item	SER
L286	1	E170	1	Q120	1
T267	2	T171	1	Y121	1
V268	3	G172	2	A122	1
P269	4	G173	2	I123	1
A270	5	T174	1	V124	1
K271	6	A175	1	Q125	1
P272	7	T176	1	A126	1
D273	8	Q177	1	R127	1
L276	9	T178	1	I132	1
T277	10	I181	1	D133	1
I278	11	L182	1	K134	1
W281	12	L185	1	P137	1
T282	13	G189	1	L138	1
L283	14	M190	1	V144	1
L284	15	T204	1	L150	1
P285	16	R207	1	L151	1
G286	17	L210	1	D152	1
V287	18	T219	1	L153	1
R292	19	A220	1	P156	1
T293	20	L223	1	D157	1
L294	21	R224	1	V158	1
L298	22	M227	1	V159	1
N302	23	N228	1	Q162	1
A303	24	T229	1	S163	1
D304	25	A230	1	E164	1
L307	26	K231	1	Y165	1
K308	27	D232	1	L166	1
P309	28	N233	1	I167	1
N312	29	V234	1		
L315	30	V235	1		
THR	31	A236	1		
HIS	32	K237	1		
ALA	33	D242	1		
HIS	34	P243	1		
HIS	35	T247	1		
HIS	36	I250	1		
HIS	37	S253	1		
HIS	38	T254	1		
HIS	39	A255	1		
HIS	40	V256	1		
HIS	41	L257	1		
HIS	42	D260	1		
HIS	43	T264	1		
HIS	44	T265	1		
D345	45	Q339	1		
R349	46	R340	1		
P352	47	V341	1		
K353	48	I342	1		
R354	49	T343	1		
V357	50	W344	1		
F358	51				
Q359	52				
A360	53				
T365	54				
A366	55				
L367	56				
R368	57				
E375	58				
V378	59				
L382	60				
F383	61				
L384	62				
I385	63				
E388	64				
A389	65				
A394	66				
L395	67				
E396	68				
R397	69				
S402	70				

- Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	159.79Å 159.79Å 683.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 3.37 49.12 – 3.37	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.12-3.37) 99.4 (49.12-3.37)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.248 , 0.286 0.241 , 0.274	Depositor DCC
R_{free} test set	2415 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	B	0.22	0/2498	0.42	0/3401
1	C	0.22	0/2513	0.42	0/3421
2	A	0.21	0/8089	0.40	0/11015
All	All	0.21	0/13100	0.41	0/17837

There are no bond length outliers.

There are no bond angle outliers.

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	B	2458	0	2522	118	0
1	C	2473	0	2533	103	0
2	A	7923	0	8166	408	0
3	A	1	0	0	0	0
4	A	7	0	0	0	0
4	B	4	0	0	0	0
4	C	10	0	0	0	0
All	All	12876	0	13221	600	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 23.

All (600) 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:C:256:TRP:CZ3	1:C:257:LEU:HD12	1.45	1.48
2:A:661:LEU:HD23	2:A:662:TRP:N	1.45	1.29
1:C:256:TRP:CZ3	1:C:257:LEU:CD1	2.34	1.11
1:B:120:GLN:HE22	1:B:243:PRO:HD2	1.17	1.05
1:C:256:TRP:CH2	1:C:257:LEU:CD1	2.44	1.01
2:A:550:VAL:HG13	2:A:913:TRP:CD1	1.96	1.01
2:A:550:VAL:HG13	2:A:913:TRP:HD1	1.24	1.00
2:A:661:LEU:HD23	2:A:661:LEU:C	1.81	0.99
1:C:256:TRP:CH2	1:C:257:LEU:HD12	1.97	0.98
2:A:660:ASN:ND2	2:A:660:ASN:H	1.65	0.94
2:A:48:ILE:HD11	2:A:131:PRO:HD2	1.47	0.94
2:A:661:LEU:C	2:A:661:LEU:CD2	2.35	0.94
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.48	0.93
2:A:550:VAL:HA	2:A:913:TRP:HE1	1.30	0.93
2:A:944:MET:HG2	2:A:980:ARG:HD3	1.52	0.92
2:A:660:ASN:HD22	2:A:660:ASN:N	1.64	0.91
2:A:298:ARG:HE	2:A:328:SER:HB2	1.36	0.90
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.53	0.90
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.55	0.89
2:A:950:HIS:HA	2:A:953:GLU:HG2	1.54	0.88
1:B:174:THR:H	1:B:177:GLN:HE21	1.18	0.87
1:C:181:ILE:HG22	1:C:182:LEU:HD12	1.57	0.86
2:A:660:ASN:HD22	2:A:660:ASN:H	0.89	0.86
2:A:904:VAL:HG23	2:A:905:PRO:HD3	1.59	0.85
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.61	0.83
2:A:961:PRO:HA	2:A:1043:HIS:HE1	1.44	0.83
2:A:240:LEU:HD21	2:A:267:ILE:HD11	1.58	0.83
2:A:661:LEU:CD2	2:A:662:TRP:N	2.37	0.83
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.44	0.82
2:A:661:LEU:HD21	2:A:663:VAL:HG13	1.61	0.81
2:A:365:VAL:HG11	2:A:501:MET:HB3	1.63	0.80
2:A:973:LEU:HD21	2:A:1036:LYS:HB3	1.64	0.79
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.66	0.78
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.65	0.77
2:A:48:ILE:HD13	2:A:48:ILE:H	1.47	0.77
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.65	0.77
1:C:302:ASN:HD21	1:C:307:LEU:H	1.31	0.77
1:B:120:GLN:NE2	1:B:243:PRO:HD2	1.98	0.76
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.67	0.76
2:A:969:LEU:HD21	2:A:1036:LYS:HB2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:891:PHE:HE2	2:A:942:VAL:HG13	1.52	0.75
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.69	0.74
1:B:204:ILE:HD12	1:B:204:ILE:H	1.51	0.74
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.21	0.74
2:A:712:SER:HB3	2:A:827:ASP:HB3	1.69	0.74
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.69	0.74
2:A:980:ARG:NH1	2:A:1028:LEU:HA	2.02	0.74
2:A:940:PHE:HE1	2:A:984:LYS:HG2	1.51	0.74
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.67	0.74
1:B:117:ASN:HD22	1:B:119:TYR:H	1.32	0.73
2:A:51:THR:HG23	2:A:127:ALA:HA	1.70	0.73
1:B:223:LEU:HD12	1:B:235:VAL:HG12	1.71	0.73
2:A:270:GLU:HG2	2:A:271:MET:H	1.54	0.72
2:A:365:VAL:HB	2:A:411:ILE:HD11	1.72	0.72
2:A:532:VAL:HG21	2:A:1029:PHE:HB3	1.72	0.71
1:C:132:ILE:HD11	1:C:229:ILE:HB	1.72	0.71
2:A:400:VAL:HA	2:A:403:MET:HG3	1.74	0.70
2:A:26:TRP:HD1	2:A:379:ILE:HD13	1.57	0.70
2:A:42:LEU:H	2:A:42:LEU:HD12	1.57	0.70
2:A:141:GLU:HG2	2:A:288:VAL:HG12	1.75	0.69
2:A:456:ILE:HG12	2:A:886:LEU:HD13	1.73	0.69
2:A:955:VAL:HG13	2:A:956:PRO:HD3	1.75	0.69
2:A:418:LEU:HG	2:A:438:VAL:HG21	1.75	0.69
1:B:104:LEU:HD22	1:B:361:SER:HB3	1.75	0.69
2:A:701:GLU:HG2	2:A:705:ARG:HH22	1.56	0.68
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.74	0.68
2:A:153:LEU:H	2:A:153:LEU:HD12	1.57	0.68
2:A:237:LEU:HG	2:A:243:PHE:CE1	2.29	0.68
2:A:61:VAL:O	2:A:65:VAL:HG12	1.93	0.68
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.24	0.68
1:B:280:LYS:HA	1:B:280:LYS:HE3	1.76	0.67
1:B:93:GLY:HA3	2:A:146:ASP:O	1.94	0.67
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.77	0.67
2:A:550:VAL:HG12	2:A:909:VAL:HG22	1.76	0.67
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.29	0.66
1:C:339:GLN:HG3	1:C:357:VAL:HG23	1.76	0.66
2:A:364:LEU:O	2:A:368:ILE:HG12	1.94	0.66
2:A:893:ARG:HB3	2:A:896:GLU:HB2	1.78	0.66
1:B:117:ASN:ND2	1:B:119:TYR:H	1.93	0.66
2:A:466:THR:O	2:A:871:LYS:HE2	1.96	0.65
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:O	1:C:256:TRP:N	2.30	0.65
2:A:413:ASN:O	2:A:417:ARG:HB2	1.97	0.65
2:A:1024:PRO:O	2:A:1028:LEU:HG	1.97	0.65
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.78	0.64
2:A:715:ALA:HB2	2:A:824:ILE:HG12	1.80	0.64
2:A:550:VAL:HG11	2:A:909:VAL:HG13	1.78	0.64
1:C:256:TRP:CE3	1:C:257:LEU:HD12	2.25	0.64
2:A:330:LEU:HD22	2:A:567:GLU:HB3	1.79	0.63
1:B:84:ILE:HG12	1:B:85:ASP:N	2.13	0.63
2:A:315:LEU:HD11	2:A:321:ILE:HD11	1.80	0.63
2:A:475:PHE:HZ	2:A:562:LEU:HD21	1.63	0.63
2:A:572:TYR:HE2	2:A:592:THR:HG21	1.64	0.63
1:C:126:ALA:HB2	1:C:229:ILE:HD11	1.80	0.63
2:A:452:ILE:O	2:A:456:ILE:HG13	1.98	0.63
2:A:529:LEU:O	2:A:532:VAL:HG12	1.99	0.62
2:A:38:ALA:HB2	2:A:331:ILE:HD13	1.81	0.62
2:A:685:VAL:HG11	2:A:696:MET:HB3	1.81	0.62
2:A:729:ASN:ND2	2:A:732:LYS:H	1.96	0.62
1:B:114:VAL:HG12	1:B:309:PRO:HA	1.80	0.62
2:A:359:HIS:CD2	2:A:361:ARG:H	2.17	0.62
2:A:961:PRO:HA	2:A:1043:HIS:CE1	2.31	0.62
1:B:335:THR:HG22	1:B:391:ILE:HD12	1.80	0.62
2:A:377:ALA:O	2:A:381:MET:HG3	1.99	0.62
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.82	0.62
1:B:360:ALA:HB2	1:B:365:THR:HG22	1.81	0.62
1:C:165:TYR:CE2	1:C:182:LEU:HD11	2.35	0.62
2:A:140:TYR:HE1	2:A:323:THR:HG1	1.46	0.61
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.30	0.61
2:A:456:ILE:HA	2:A:886:LEU:HD13	1.82	0.61
2:A:525:TYR:HE2	2:A:1029:PHE:HE2	1.48	0.61
1:C:287:VAL:HB	1:C:294:LEU:HD23	1.82	0.61
2:A:877:PRO:O	2:A:881:MET:HG2	2.00	0.61
1:C:126:ALA:HB2	1:C:229:ILE:CD1	2.30	0.61
2:A:297:ALA:O	2:A:301:ILE:HG13	2.01	0.61
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.82	0.61
2:A:243:PHE:HB3	2:A:265:VAL:HG21	1.81	0.61
1:C:388:GLU:HB2	2:A:657:GLY:H	1.66	0.61
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.01	0.60
2:A:999:LEU:HD23	2:A:1017:ILE:HD12	1.82	0.60
1:B:385:ILE:HG22	1:B:389:ALA:HB2	1.83	0.60
2:A:409:VAL:HG11	2:A:450:LEU:HD21	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:572:TYR:CE2	2:A:592:THR:HG21	2.36	0.60
2:A:488:GLY:O	2:A:492:LEU:HB2	2.01	0.60
1:C:80:SER:HA	1:C:397:ARG:HD2	1.83	0.60
2:A:6:ILE:HG21	2:A:444:VAL:HG22	1.82	0.60
2:A:20:ALA:HA	2:A:23:LEU:HB3	1.84	0.60
2:A:122:PRO:O	2:A:125:VAL:HG22	2.02	0.60
2:A:876:VAL:O	2:A:879:THR:HG22	2.02	0.60
2:A:536:PRO:HB2	2:A:1037:LEU:HD12	1.84	0.60
1:B:89:THR:H	2:A:590:GLN:HE22	1.49	0.59
2:A:861:GLN:HA	2:A:864:LEU:HD12	1.84	0.59
2:A:880:LEU:O	2:A:883:ILE:HG22	2.03	0.59
2:A:642:MET:HA	2:A:642:MET:HE3	1.85	0.59
1:B:307:LEU:HD12	1:B:307:LEU:H	1.67	0.59
2:A:270:GLU:HG2	2:A:271:MET:N	2.17	0.59
2:A:141:GLU:HB2	2:A:325:TYR:HB3	1.84	0.59
1:C:359:GLN:HG3	1:C:360:ALA:N	2.18	0.59
2:A:786:LEU:HB3	2:A:798:LEU:HB2	1.84	0.58
1:B:123:ILE:HB	1:C:227:MET:CG	2.33	0.58
2:A:729:ASN:HB3	2:A:732:LYS:HB2	1.85	0.58
1:C:151:LEU:HD11	1:C:210:LEU:HD12	1.85	0.58
1:B:94:VAL:HG12	1:B:96:THR:HG23	1.86	0.58
2:A:883:ILE:O	2:A:887:LEU:HG	2.02	0.58
2:A:980:ARG:HH12	2:A:1028:LEU:HA	1.67	0.58
2:A:440:THR:O	2:A:444:VAL:HG23	2.03	0.58
2:A:458:THR:HB	2:A:483:THR:HG23	1.84	0.58
2:A:661:LEU:HD23	2:A:662:TRP:CA	2.31	0.58
2:A:535:TRP:NE1	2:A:537:LYS:HB3	2.18	0.58
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.86	0.58
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.04	0.57
1:C:317:LEU:C	1:C:317:LEU:HD12	2.24	0.57
1:B:385:ILE:HG13	2:A:272:ARG:HB2	1.86	0.57
1:B:378:VAL:HG21	1:B:383:PHE:CE2	2.38	0.57
2:A:411:ILE:HG23	2:A:415:HIS:CE1	2.40	0.57
2:A:701:GLU:HG2	2:A:705:ARG:NH2	2.19	0.57
2:A:186:GLU:HG3	2:A:767:PRO:HG2	1.85	0.57
1:C:163:SER:HB3	1:C:204:ILE:HD11	1.86	0.57
1:C:384:LEU:HD11	2:A:588:MET:HE2	1.85	0.57
2:A:22:PHE:HA	2:A:25:ILE:HG22	1.86	0.57
2:A:402:ALA:HA	2:A:405:ASP:HB3	1.87	0.57
2:A:786:LEU:HD22	2:A:787:PRO:HD2	1.85	0.57
1:B:358:PHE:HE2	1:C:273:ASP:HB3	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:475:PHE:CZ	2:A:562:LEU:HD21	2.39	0.56
2:A:365:VAL:HG21	2:A:501:MET:HA	1.87	0.56
2:A:384:GLN:HG3	2:A:386:LEU:HD13	1.87	0.56
1:B:174:THR:H	1:B:177:GLN:NE2	1.95	0.56
2:A:399:ALA:HB2	2:A:482:LYS:HG2	1.88	0.56
2:A:872:LEU:O	2:A:876:VAL:HG23	2.05	0.56
1:B:123:ILE:HB	1:C:227:MET:HG2	1.87	0.56
2:A:550:VAL:HA	2:A:913:TRP:NE1	2.10	0.56
1:B:332:LEU:HA	1:B:341:VAL:HG12	1.86	0.56
1:C:174:THR:HG22	1:C:176:THR:H	1.70	0.56
2:A:574:PRO:HA	2:A:660:ASN:HA	1.88	0.56
2:A:522:ILE:O	2:A:526:HIS:HD2	1.87	0.56
2:A:660:ASN:ND2	2:A:660:ASN:N	2.30	0.56
1:B:386:ASP:HB2	2:A:269:PRO:O	2.05	0.56
2:A:40:PRO:O	2:A:42:LEU:HG	2.06	0.55
2:A:661:LEU:HD12	2:A:679:SER:HB3	1.88	0.55
1:B:80:SER:HB3	1:B:82:VAL:HG12	1.88	0.55
1:C:330:GLN:O	1:C:382:LEU:HD12	2.07	0.55
2:A:340:GLY:O	2:A:344:GLU:HG2	2.06	0.55
2:A:413:ASN:HD22	2:A:442:ALA:HB1	1.70	0.55
2:A:732:LYS:HB3	2:A:801:VAL:HA	1.89	0.55
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.89	0.55
2:A:690:LEU:HD11	2:A:813:LEU:HD11	1.89	0.55
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.05	0.55
1:C:268:VAL:HG12	1:C:276:LEU:HD11	1.89	0.55
2:A:572:TYR:HE1	2:A:660:ASN:HB2	1.71	0.55
1:C:359:GLN:HG3	1:C:360:ALA:H	1.72	0.54
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.37	0.54
2:A:361:ARG:O	2:A:365:VAL:HG23	2.07	0.54
1:C:332:LEU:HD11	1:C:357:VAL:HG22	1.88	0.54
1:C:345:ASP:HB2	1:C:349:ARG:O	2.07	0.54
1:C:352:PRO:HG3	1:C:395:LEU:HD12	1.88	0.54
2:A:422:GLN:HG2	2:A:427:ASP:OD1	2.07	0.54
1:B:336:GLY:HA3	2:A:775:SER:OG	2.08	0.54
2:A:960:ASN:N	2:A:961:PRO:HD2	2.22	0.54
2:A:595:LEU:O	2:A:598:SER:HB3	2.07	0.54
2:A:904:VAL:HG12	2:A:937:ALA:HB3	1.90	0.54
2:A:349:VAL:HG11	2:A:404:VAL:HG11	1.89	0.54
1:C:120:GLN:OE1	1:C:243:PRO:HD2	2.08	0.54
1:C:158:TRP:O	1:C:162:GLN:HG3	2.08	0.54
2:A:243:PHE:O	2:A:246:ILE:HG13	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:715:ALA:CB	2:A:824:ILE:HG12	2.37	0.54
2:A:223:GLU:O	2:A:224:LEU:HD23	2.08	0.53
2:A:291:LEU:HD22	2:A:297:ALA:HA	1.89	0.53
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.08	0.53
1:B:245:TRP:CE3	1:B:297:ARG:HD3	2.43	0.53
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.88	0.53
2:A:453:SER:HA	2:A:456:ILE:HD12	1.90	0.53
1:B:124:VAL:O	1:B:235:VAL:HG22	2.08	0.53
1:C:138:LEU:HD21	1:C:144:VAL:HG11	1.90	0.53
2:A:871:LYS:O	2:A:875:MET:HB2	2.09	0.53
2:A:217:ALA:HB3	2:A:233:ALA:HB3	1.89	0.53
2:A:404:VAL:HG22	2:A:408:ILE:HG23	1.91	0.53
2:A:474:LEU:O	2:A:477:PRO:HD2	2.08	0.53
1:B:164:GLU:O	1:B:168:LEU:HD13	2.08	0.53
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.39	0.53
1:B:252:GLU:CG	1:C:270:ALA:HB2	2.39	0.53
1:B:287:VAL:HG12	1:B:294:LEU:HD23	1.90	0.53
1:C:342:ILE:HB	1:C:378:VAL:HG12	1.90	0.53
1:B:250:ILE:HG21	1:B:258:VAL:HG11	1.91	0.53
1:B:274:LYS:O	1:B:276:LEU:HD23	2.09	0.53
2:A:13:ARG:HA	2:A:499:ILE:HD13	1.90	0.53
2:A:140:TYR:HD2	2:A:304:VAL:HG11	1.73	0.53
2:A:432:ASN:HA	2:A:435:ARG:HG2	1.90	0.53
2:A:940:PHE:CE1	2:A:984:LYS:HG2	2.39	0.52
2:A:991:ILE:HG21	2:A:1020:MET:SD	2.49	0.52
2:A:118:GLN:HE22	2:A:126:SER:HA	1.75	0.52
1:B:174:THR:HG22	1:B:176:THR:H	1.75	0.52
1:C:124:VAL:HB	1:C:235:VAL:HG13	1.92	0.52
1:B:255:ALA:HB3	1:C:270:ALA:HB1	1.91	0.52
2:A:69:LEU:HD11	2:A:121:LEU:HD11	1.91	0.52
2:A:184:VAL:HG23	2:A:270:GLU:HB3	1.91	0.52
1:B:271:ARG:CD	1:B:306:ALA:HB1	2.39	0.52
2:A:882:ILE:O	2:A:886:LEU:HG	2.10	0.52
2:A:97:PHE:CZ	2:A:106:ALA:HB1	2.44	0.52
2:A:519:ARG:O	2:A:523:ARG:HG3	2.10	0.52
2:A:534:HIS:C	2:A:534:HIS:CD2	2.83	0.52
2:A:620:PRO:HB2	2:A:622:GLU:HG3	1.92	0.52
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.75	0.52
2:A:436:TRP:C	2:A:436:TRP:CD1	2.83	0.51
2:A:49:ILE:HB	2:A:93:VAL:HB	1.92	0.51
2:A:275:ILE:CD1	2:A:586:ALA:HB2	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:661:LEU:HD22	2:A:661:LEU:C	2.29	0.51
1:C:166:LEU:O	1:C:170:GLU:HG2	2.10	0.51
1:B:307:LEU:N	1:B:307:LEU:HD12	2.25	0.51
1:C:106:PHE:O	1:C:318:ASN:HA	2.10	0.51
1:B:132:ILE:HD11	1:B:229:ILE:HB	1.92	0.51
1:B:158:TRP:O	1:B:162:GLN:HG3	2.10	0.51
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.93	0.51
2:A:1028:LEU:O	2:A:1032:PRO:HG2	2.10	0.51
2:A:421:TRP:O	2:A:425:HIS:HB2	2.10	0.51
2:A:554:LEU:HD21	2:A:912:ILE:HG12	1.93	0.51
2:A:446:VAL:HG12	2:A:946:MET:HE3	1.93	0.51
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.46	0.51
1:C:298:LEU:HD11	1:C:315:LEU:HD13	1.92	0.51
2:A:327:ARG:NH1	2:A:666:ILE:HG12	2.26	0.51
1:C:256:TRP:CH2	1:C:257:LEU:HD13	2.38	0.51
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.92	0.51
2:A:420:GLU:HG3	2:A:421:TRP:N	2.25	0.51
1:C:388:GLU:HB2	2:A:657:GLY:N	2.26	0.51
1:C:327:ILE:HD13	1:C:367:LEU:HD21	1.93	0.51
2:A:74:LEU:HD11	2:A:817:ASN:HA	1.93	0.50
2:A:906:PHE:O	2:A:909:VAL:HG12	2.11	0.50
1:C:302:ASN:ND2	1:C:307:LEU:H	2.03	0.50
2:A:342:LEU:HD21	2:A:397:ALA:HA	1.92	0.50
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.92	0.50
1:B:104:LEU:HD11	1:B:359:GLN:O	2.12	0.50
1:C:223:LEU:C	1:C:224:ARG:HD2	2.32	0.50
2:A:49:ILE:HD11	2:A:73:MET:HE3	1.94	0.50
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.92	0.50
1:C:384:LEU:HD21	2:A:588:MET:HE2	1.93	0.50
2:A:764:ALA:O	2:A:765:ARG:HG3	2.11	0.50
2:A:925:ALA:O	2:A:1012:ILE:HG13	2.11	0.50
2:A:992:ILE:O	2:A:996:LEU:HB2	2.11	0.50
1:B:391:ILE:HG13	2:A:774:GLN:OE1	2.12	0.50
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.47	0.50
2:A:837:VAL:O	2:A:841:GLN:HG3	2.11	0.50
1:B:162:GLN:OE1	1:B:198:LEU:HD13	2.10	0.50
1:B:174:THR:HB	1:B:177:GLN:HG3	1.93	0.50
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.94	0.50
1:B:356:ALA:HB1	1:B:368:ARG:NH1	2.27	0.50
2:A:546:SER:O	2:A:550:VAL:HG23	2.11	0.50
2:A:56:GLN:HB3	2:A:60:ILE:HG23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:690:LEU:HD22	2:A:718:LEU:CD2	2.41	0.50
2:A:950:HIS:HA	2:A:953:GLU:CG	2.34	0.50
2:A:984:LYS:HG3	2:A:1028:LEU:HD21	1.94	0.49
2:A:667:ARG:HH11	2:A:861:GLN:HE22	1.60	0.49
1:C:124:VAL:O	1:C:235:VAL:HG12	2.11	0.49
2:A:408:ILE:HD12	2:A:986:MET:HB3	1.93	0.49
1:B:94:VAL:HG21	1:B:350:PHE:HZ	1.76	0.49
2:A:122:PRO:HB2	2:A:125:VAL:HG13	1.93	0.49
2:A:291:LEU:HD13	2:A:300:VAL:HG11	1.94	0.49
2:A:744:GLN:O	2:A:748:THR:HG23	2.12	0.49
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.48	0.49
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.11	0.49
1:B:339:GLN:HG3	1:B:357:VAL:HG22	1.94	0.49
1:C:254:ILE:O	1:C:255:ALA:C	2.51	0.49
2:A:153:LEU:CD1	2:A:153:LEU:H	2.24	0.49
2:A:956:PRO:HA	2:A:959:ASN:ND2	2.27	0.49
2:A:276:ALA:HB3	2:A:284:VAL:O	2.12	0.49
2:A:46:GLN:HG2	2:A:134:THR:HG22	1.94	0.49
2:A:143:ALA:HB2	2:A:606:PHE:HE1	1.77	0.49
2:A:402:ALA:HB3	2:A:486:MET:CE	2.42	0.49
2:A:411:ILE:HG12	2:A:501:MET:HE3	1.93	0.49
2:A:550:VAL:HG12	2:A:550:VAL:O	2.11	0.49
2:A:83:ARG:HG2	2:A:816:GLU:HG3	1.94	0.49
1:B:340:ARG:HD3	1:B:395:LEU:HD12	1.94	0.49
1:C:110:PHE:CE1	1:C:250:ILE:HG13	2.47	0.49
2:A:455:LEU:HD13	2:A:455:LEU:O	2.12	0.49
1:B:223:LEU:C	1:B:224:ARG:HD2	2.33	0.49
1:B:280:LYS:HE3	1:B:281:TRP:H	1.77	0.49
1:B:144:VAL:HG21	1:B:238:ILE:HD13	1.95	0.49
1:B:125:GLN:NE2	1:C:228:ASN:H	2.10	0.49
2:A:42:LEU:HD13	2:A:670:ILE:HD13	1.95	0.49
2:A:868:ALA:O	2:A:872:LEU:HG	2.13	0.49
2:A:143:ALA:HB2	2:A:606:PHE:CE1	2.48	0.48
1:B:153:LEU:N	1:B:153:LEU:HD23	2.28	0.48
1:B:195:ILE:O	1:B:198:LEU:HB3	2.13	0.48
2:A:910:GLY:HA3	2:A:1022:THR:OG1	2.12	0.48
2:A:403:MET:SD	2:A:485:ALA:HB1	2.53	0.48
2:A:601:GLU:OE2	2:A:637:ARG:HD3	2.13	0.48
2:A:969:LEU:O	2:A:973:LEU:HD13	2.13	0.48
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.43	0.48
2:A:395:GLY:HA2	2:A:398:ILE:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:522:ILE:HG23	2:A:526:HIS:HE2	1.79	0.48
2:A:56:GLN:HB3	2:A:60:ILE:CG2	2.43	0.48
1:B:344:VAL:HG13	1:B:348:GLY:HA2	1.94	0.48
2:A:419:GLU:O	2:A:423:HIS:HD2	1.96	0.48
2:A:898:LEU:C	2:A:898:LEU:HD23	2.34	0.48
1:B:222:ASP:HB2	1:B:234:VAL:O	2.13	0.48
1:B:271:ARG:NE	1:B:306:ALA:HB1	2.28	0.48
2:A:461:PHE:CZ	2:A:464:ILE:HD12	2.49	0.48
2:A:608:LYS:HE2	2:A:625:GLU:HG2	1.95	0.48
1:B:117:ASN:HD22	1:B:117:ASN:C	2.16	0.48
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.44	0.48
2:A:114:LEU:HD11	2:A:127:ALA:HB1	1.94	0.48
2:A:550:VAL:CG1	2:A:909:VAL:HG22	2.43	0.48
2:A:368:ILE:O	2:A:368:ILE:HG22	2.14	0.48
2:A:376:ILE:HD13	2:A:488:GLY:HA2	1.96	0.48
2:A:842:LYS:O	2:A:846:GLU:HG2	2.14	0.48
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.44	0.48
2:A:644:LYS:HB3	2:A:644:LYS:NZ	2.29	0.48
2:A:525:TYR:CE1	2:A:977:ALA:HB1	2.49	0.48
2:A:37:ASP:OD2	2:A:297:ALA:HB3	2.14	0.47
2:A:48:ILE:HG22	2:A:94:TYR:CD2	2.49	0.47
2:A:700:ILE:HA	2:A:703:VAL:HG22	1.95	0.47
2:A:952:ILE:HA	2:A:957:SER:CB	2.44	0.47
1:B:360:ALA:HA	1:B:365:THR:HA	1.95	0.47
2:A:525:TYR:CE2	2:A:1029:PHE:HE2	2.31	0.47
2:A:185:LYS:HG2	2:A:766:TYR:CD2	2.49	0.47
2:A:324:THR:HG21	2:A:606:PHE:CD1	2.48	0.47
2:A:57:ALA:O	2:A:61:VAL:HG23	2.14	0.47
2:A:630:LEU:HD13	2:A:642:MET:HE1	1.96	0.47
2:A:965:SER:HB2	2:A:968:LYS:HB2	1.96	0.47
1:B:252:GLU:HG2	1:C:270:ALA:HB2	1.97	0.47
1:B:322:GLU:O	1:B:324:MET:HG3	2.14	0.47
1:B:386:ASP:O	1:B:387:SER:C	2.53	0.47
2:A:482:LYS:O	2:A:486:MET:HG2	2.14	0.47
2:A:376:ILE:HD13	2:A:488:GLY:CA	2.45	0.47
2:A:604:ARG:HB2	2:A:629:GLN:HE21	1.79	0.47
2:A:456:ILE:HG12	2:A:886:LEU:CD1	2.44	0.47
2:A:48:ILE:HG12	2:A:130:GLY:HA3	1.95	0.47
2:A:666:ILE:O	2:A:670:ILE:HG13	2.14	0.47
2:A:76:VAL:HG13	2:A:77:PRO:HD2	1.95	0.47
2:A:995:LEU:C	2:A:1017:ILE:HD11	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:VAL:HG11	2:A:103:PRO:HA	1.97	0.47
2:A:139:ILE:O	2:A:325:TYR:HD1	1.97	0.47
2:A:240:LEU:HD22	2:A:265:VAL:HG12	1.97	0.47
2:A:291:LEU:HD21	2:A:295:LYS:O	2.15	0.47
2:A:431:ASP:CG	2:A:432:ASN:H	2.18	0.47
2:A:988:VAL:O	2:A:988:VAL:HG12	2.15	0.47
1:C:389:ALA:O	1:C:394:ALA:HB3	2.15	0.47
2:A:392:SER:O	2:A:396:ILE:HG13	2.15	0.47
1:B:358:PHE:CD2	1:C:272:PRO:HB2	2.50	0.47
2:A:42:LEU:HD12	2:A:42:LEU:N	2.25	0.47
1:B:143:LYS:HD2	1:B:216:GLY:O	2.15	0.47
1:B:291:THR:O	1:B:293:THR:N	2.48	0.47
2:A:1037:LEU:HD23	2:A:1037:LEU:O	2.16	0.46
2:A:571:LEU:HD23	2:A:627:THR:HA	1.97	0.46
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.97	0.46
2:A:459:LEU:HB3	2:A:882:ILE:HD13	1.98	0.46
2:A:296:ASN:HB3	2:A:299:GLU:HB3	1.97	0.46
2:A:573:MET:HA	2:A:624:VAL:O	2.15	0.46
2:A:729:ASN:C	2:A:729:ASN:HD22	2.19	0.46
2:A:771:ARG:HD2	2:A:777:ARG:NE	2.31	0.46
2:A:985:ALA:O	2:A:989:ALA:HB2	2.15	0.46
1:C:223:LEU:HD21	1:C:233:ASN:HD22	1.80	0.46
2:A:637:ARG:HH11	2:A:637:ARG:HB2	1.79	0.46
2:A:497:ILE:HB	2:A:498:PRO:HD3	1.96	0.46
2:A:551:LEU:HD23	2:A:551:LEU:C	2.35	0.46
2:A:620:PRO:HB2	2:A:622:GLU:CG	2.45	0.46
2:A:771:ARG:HG3	2:A:772:TYR:N	2.29	0.46
2:A:952:ILE:HG12	2:A:1039:TRP:HE1	1.80	0.46
1:C:266:LEU:HG	1:C:278:ILE:HD11	1.98	0.46
2:A:65:VAL:HA	2:A:121:LEU:HD22	1.98	0.46
2:A:137:GLY:O	2:A:290:ILE:HA	2.15	0.46
2:A:813:LEU:HA	2:A:813:LEU:HD13	1.81	0.46
1:B:372:ALA:HB3	1:B:375:GLU:HG3	1.98	0.46
1:C:94:VAL:HG21	1:C:385:ILE:HD11	1.97	0.46
2:A:297:ALA:O	2:A:300:VAL:HG12	2.16	0.46
2:A:298:ARG:O	2:A:298:ARG:HD3	2.15	0.46
1:C:91:ASN:O	2:A:591:LYS:HD3	2.16	0.46
1:C:223:LEU:HD12	1:C:235:VAL:HB	1.98	0.46
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.16	0.46
2:A:580:ILE:HG22	2:A:622:GLU:HB3	1.97	0.46
2:A:454:LEU:HA	2:A:457:ILE:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:467:LEU:O	2:A:472:GLY:HA3	2.16	0.45
2:A:625:GLU:HG3	2:A:625:GLU:O	2.16	0.45
2:A:884:PHE:CD1	2:A:884:PHE:C	2.90	0.45
2:A:446:VAL:HG12	2:A:946:MET:CE	2.46	0.45
1:B:271:ARG:HD2	1:B:306:ALA:HB1	1.98	0.45
2:A:279:ASN:ND2	2:A:605:VAL:H	2.14	0.45
1:C:332:LEU:HA	1:C:341:VAL:HG12	1.98	0.45
2:A:408:ILE:HG13	2:A:409:VAL:N	2.32	0.45
2:A:740:VAL:O	2:A:744:GLN:HG3	2.16	0.45
1:B:390:ASN:HA	2:A:774:GLN:HE22	1.81	0.45
2:A:153:LEU:N	2:A:153:LEU:HD12	2.26	0.45
1:B:84:ILE:CD1	2:A:594:LYS:HB2	2.47	0.45
2:A:984:LYS:HD2	2:A:984:LYS:C	2.37	0.45
1:B:196:ARG:O	1:B:199:ILE:HG12	2.16	0.45
2:A:31:ILE:HG13	2:A:378:PHE:CZ	2.51	0.45
2:A:53:TYR:CE1	2:A:56:GLN:HG3	2.51	0.45
2:A:991:ILE:O	2:A:995:LEU:HD13	2.17	0.45
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.41	0.45
2:A:575:SER:O	2:A:658:LEU:HD12	2.16	0.45
2:A:661:LEU:HD23	2:A:662:TRP:H	1.63	0.45
2:A:67:TYR:N	2:A:68:PRO:HD2	2.31	0.45
1:B:220:ALA:HB3	1:B:237:LYS:HB3	1.99	0.45
1:B:123:ILE:HD12	1:B:237:LYS:HG3	1.99	0.45
2:A:404:VAL:O	2:A:408:ILE:HG12	2.17	0.45
2:A:462:ILE:N	2:A:463:PRO:CD	2.80	0.45
1:B:302:ASN:HD21	1:B:306:ALA:N	2.15	0.45
2:A:637:ARG:HB2	2:A:640:MET:HG3	1.99	0.45
2:A:816:GLU:O	2:A:817:ASN:HB2	2.17	0.45
2:A:988:VAL:HG11	2:A:1024:PRO:HG2	1.99	0.45
1:C:114:VAL:HG12	1:C:309:PRO:HA	1.99	0.45
2:A:988:VAL:CG1	2:A:1024:PRO:HG2	2.46	0.45
2:A:117:VAL:HG12	2:A:117:VAL:O	2.16	0.45
2:A:38:ALA:O	2:A:390:ILE:HG22	2.17	0.45
2:A:42:LEU:HB3	2:A:470:GLN:HG3	1.99	0.45
2:A:222:ILE:HG23	2:A:229:TYR:HB2	1.98	0.44
2:A:494:ILE:O	2:A:494:ILE:HG12	2.17	0.44
2:A:723:TYR:O	2:A:806:VAL:HA	2.17	0.44
2:A:561:PHE:CE1	2:A:864:LEU:HB3	2.51	0.44
2:A:944:MET:HG2	2:A:980:ARG:CD	2.37	0.44
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.41	0.44
1:C:358:PHE:HD2	1:C:368:ARG:NH2	2.14	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:359:HIS:HD2	2:A:360:VAL:N	2.14	0.44
2:A:6:ILE:O	2:A:6:ILE:HD13	2.17	0.44
2:A:980:ARG:C	2:A:983:PRO:HD2	2.36	0.44
1:C:384:LEU:HD21	2:A:588:MET:CE	2.48	0.44
2:A:255:VAL:HA	2:A:256:PRO:HD3	1.82	0.44
2:A:453:SER:O	2:A:456:ILE:HB	2.18	0.44
2:A:571:LEU:HB3	2:A:573:MET:HE2	2.00	0.44
2:A:876:VAL:HB	2:A:877:PRO:HD3	2.00	0.44
1:C:134:LYS:HB3	1:C:152:ASP:HB2	1.98	0.44
1:C:156:PRO:O	1:C:159:VAL:HG22	2.17	0.44
2:A:526:HIS:N	2:A:527:PRO:CD	2.81	0.44
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.99	0.44
2:A:837:VAL:HG21	2:A:862:PHE:CD2	2.52	0.44
2:A:921:HIS:O	2:A:926:THR:HG21	2.18	0.44
1:B:383:PHE:C	1:B:384:LEU:HD12	2.38	0.44
2:A:525:TYR:HE1	2:A:977:ALA:HB1	1.83	0.44
1:B:252:GLU:HG3	1:C:270:ALA:HB2	2.00	0.44
2:A:599:VAL:O	2:A:602:VAL:HG13	2.18	0.44
2:A:729:ASN:HD22	2:A:732:LYS:H	1.65	0.44
2:A:193:PRO:HB3	2:A:787:PRO:HB2	2.00	0.44
1:B:385:ILE:CG2	1:B:389:ALA:HB2	2.46	0.44
2:A:27:GLY:HA3	2:A:375:CYS:HB3	2.00	0.44
2:A:28:THR:O	2:A:32:ILE:HG13	2.18	0.44
2:A:619:ALA:HB1	2:A:623:MET:HG2	2.00	0.44
1:C:171:THR:O	1:C:172:GLY:C	2.55	0.44
1:B:123:ILE:HG12	1:C:224:ARG:HB2	1.99	0.44
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.48	0.44
2:A:1020:MET:HA	2:A:1020:MET:CE	2.48	0.43
2:A:534:HIS:CD2	2:A:534:HIS:O	2.71	0.43
1:C:284:LEU:HB3	1:C:285:PRO:HD2	2.00	0.43
2:A:904:VAL:N	2:A:905:PRO:CD	2.81	0.43
2:A:1032:PRO:C	2:A:1034:ALA:H	2.22	0.43
2:A:212:ALA:C	2:A:215:GLN:HE22	2.21	0.43
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.48	0.43
1:B:85:ASP:HA	1:B:86:PRO:HD3	1.87	0.43
2:A:999:LEU:HD21	2:A:1014:ALA:HA	2.00	0.43
2:A:557:VAL:HG12	2:A:921:HIS:HA	1.99	0.43
1:B:327:ILE:CD1	1:B:341:VAL:HG11	2.48	0.43
1:C:174:THR:H	1:C:177:GLN:NE2	2.17	0.43
2:A:1001:GLY:O	2:A:1002:THR:C	2.56	0.43
2:A:636:TRP:CD1	2:A:636:TRP:N	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:746:PHE:O	2:A:750:ALA:HB3	2.18	0.43
1:B:340:ARG:HH21	1:B:354:ARG:CG	2.32	0.43
1:C:127:ARG:O	1:C:231:LYS:HE2	2.19	0.43
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.99	0.43
2:A:952:ILE:HA	2:A:957:SER:OG	2.17	0.43
2:A:272:ARG:NH2	2:A:283:GLU:OE1	2.51	0.43
2:A:575:SER:N	2:A:659:ALA:O	2.51	0.43
2:A:965:SER:HB3	2:A:968:LYS:HD3	2.01	0.43
2:A:414:ALA:HB3	2:A:501:MET:HE1	2.01	0.43
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.83	0.43
1:C:224:ARG:N	1:C:224:ARG:HD2	2.33	0.43
1:C:331:ALA:O	1:C:341:VAL:HG12	2.19	0.43
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.53	0.43
2:A:70:THR:O	2:A:74:LEU:HG	2.19	0.42
2:A:851:LYS:HB3	2:A:852:PRO:HD2	2.01	0.42
2:A:203:LEU:HD12	2:A:746:PHE:CD2	2.54	0.42
1:B:114:VAL:HG22	1:B:246:VAL:HG22	2.01	0.42
1:B:399:ARG:O	1:B:400:SER:HB2	2.19	0.42
1:C:189:GLY:O	1:C:190:MET:C	2.58	0.42
2:A:195:ARG:HD3	2:A:261:ASP:O	2.19	0.42
2:A:277:GLU:OE2	2:A:590:GLN:HG3	2.19	0.42
2:A:756:VAL:HG12	2:A:756:VAL:O	2.18	0.42
2:A:969:LEU:CD2	2:A:1036:LYS:HE3	2.48	0.42
1:B:302:ASN:HD21	1:B:307:LEU:H	1.66	0.42
2:A:590:GLN:O	2:A:594:LYS:HG3	2.19	0.42
1:B:384:LEU:HD21	1:B:395:LEU:HD23	2.01	0.42
1:C:153:LEU:HD23	1:C:153:LEU:H	1.83	0.42
1:C:268:VAL:HA	1:C:269:PRO:HD3	1.93	0.42
2:A:633:GLN:HA	2:A:636:TRP:CE2	2.54	0.42
2:A:783:LEU:O	2:A:798:LEU:HB3	2.19	0.42
1:B:259:LYS:HE3	1:B:259:LYS:HB2	1.88	0.42
1:C:86:PRO:O	1:C:90:GLN:HG3	2.19	0.42
1:C:264:PHE:HB3	1:C:315:LEU:HD11	2.02	0.42
2:A:370:LEU:HB2	2:A:371:PRO:HD3	2.02	0.42
2:A:897:ALA:O	2:A:901:ILE:HG13	2.20	0.42
2:A:927:GLY:O	2:A:931:ILE:HG12	2.20	0.42
2:A:191:ILE:HD11	2:A:206:VAL:HG11	2.01	0.42
2:A:552:TRP:N	2:A:553:PRO:CD	2.83	0.42
1:B:343:THR:HA	1:B:377:VAL:HA	2.02	0.42
1:B:384:LEU:N	1:B:384:LEU:HD12	2.35	0.42
2:A:497:ILE:O	2:A:501:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:HA	1:B:272:PRO:HD3	1.85	0.42
2:A:884:PHE:HB2	2:A:901:ILE:HD11	2.01	0.42
2:A:955:VAL:N	2:A:956:PRO:CD	2.83	0.42
1:B:307:LEU:H	1:B:307:LEU:CD1	2.33	0.42
2:A:327:ARG:O	2:A:331:ILE:HG12	2.20	0.41
2:A:381:MET:HE2	2:A:381:MET:HB2	1.83	0.41
2:A:57:ALA:HB1	2:A:58:PRO:HD2	2.01	0.41
2:A:611:LYS:HA	2:A:617:ASP:OD2	2.20	0.41
1:C:167:LEU:HD12	1:C:167:LEU:C	2.41	0.41
2:A:992:ILE:HD11	2:A:1020:MET:O	2.20	0.41
2:A:140:TYR:HE1	2:A:323:THR:OG1	2.02	0.41
2:A:994:GLY:O	2:A:997:PRO:HD2	2.20	0.41
1:B:271:ARG:HB3	1:B:274:LYS:HB2	2.02	0.41
1:C:343:THR:OG1	1:C:353:LYS:HD3	2.20	0.41
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.41
2:A:65:VAL:HA	2:A:121:LEU:CD2	2.50	0.41
2:A:121:LEU:HB3	2:A:125:VAL:HG21	2.01	0.41
2:A:342:LEU:HD23	2:A:342:LEU:HA	1.83	0.41
2:A:534:HIS:O	2:A:534:HIS:HD2	2.04	0.41
1:C:106:PHE:CZ	1:C:359:GLN:HG2	2.56	0.41
2:A:46:GLN:HB2	2:A:96:ILE:HD13	2.03	0.41
2:A:85:PHE:CD1	2:A:812:MET:HE3	2.55	0.41
1:B:132:ILE:CD1	1:B:229:ILE:HB	2.50	0.41
1:B:302:ASN:HD21	1:B:306:ALA:H	1.68	0.41
1:B:335:THR:HG23	1:B:338:GLU:O	2.21	0.41
1:C:281:TRP:HB2	1:C:298:LEU:HD23	2.02	0.41
1:C:329:SER:HA	1:C:365:THR:HG22	2.01	0.41
2:A:178:ALA:HB2	2:A:614:THR:HB	2.03	0.41
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.82	0.41
2:A:189:VAL:HG22	2:A:265:VAL:HG22	2.01	0.41
1:C:220:ALA:HB3	1:C:237:LYS:HB3	2.02	0.41
1:B:259:LYS:HG3	1:B:260:ASP:N	2.36	0.41
1:B:291:THR:O	1:B:293:THR:HG23	2.21	0.41
2:A:184:VAL:HG21	2:A:270:GLU:OE1	2.21	0.41
2:A:462:ILE:N	2:A:463:PRO:HD2	2.36	0.41
2:A:595:LEU:HB3	2:A:653:VAL:HG22	2.03	0.41
2:A:661:LEU:CD1	2:A:679:SER:HB3	2.51	0.41
1:B:308:LYS:HA	1:B:309:PRO:HD3	1.97	0.41
1:B:125:GLN:HE21	1:C:227:MET:HB3	1.85	0.41
2:A:1016:MET:HB2	2:A:1016:MET:HE2	1.91	0.41
1:B:330:GLN:NE2	2:A:267:ILE:HB	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:392:SER:O	2:A:481:THR:HG21	2.21	0.41
2:A:834:VAL:HA	2:A:837:VAL:HG22	2.02	0.41
1:B:264:PHE:HE1	1:B:281:TRP:CE2	2.39	0.41
2:A:201:ILE:HD13	2:A:248:LEU:HB3	2.02	0.41
2:A:641:THR:H	2:A:644:LYS:HB2	1.86	0.41
2:A:356:PHE:HE2	2:A:985:ALA:O	2.04	0.41
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.55	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.82	0.41
2:A:904:VAL:O	2:A:908:LEU:HG	2.20	0.40
1:C:357:VAL:HA	1:C:367:LEU:HD12	2.03	0.40
2:A:999:LEU:CD2	2:A:1017:ILE:HD12	2.49	0.40
2:A:533:LEU:HD22	2:A:1036:LYS:HD2	2.03	0.40
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.36	0.40
2:A:876:VAL:O	2:A:880:LEU:HG	2.21	0.40
2:A:590:GLN:HG2	2:A:594:LYS:HE3	2.02	0.40
2:A:899:LEU:HD22	2:A:899:LEU:HA	1.90	0.40
1:B:242:ASP:CB	1:B:243:PRO:CD	2.98	0.40
1:C:108:GLN:OE1	1:C:108:GLN:HA	2.22	0.40
1:C:322:GLU:O	1:C:324:MET:HG2	2.21	0.40
2:A:359:HIS:CD2	2:A:360:VAL:N	2.90	0.40
2:A:960:ASN:HA	2:A:963:THR:O	2.22	0.40
1:B:335:THR:HG22	1:B:391:ILE:CD1	2.48	0.40
1:C:353:LYS:HE2	1:C:375:GLU:OE2	2.21	0.40
1:C:94:VAL:CG2	1:C:385:ILE:HD11	2.51	0.40
2:A:421:TRP:O	2:A:421:TRP:HD1	2.04	0.40
2:A:834:VAL:HG22	2:A:838:HIS:HD2	1.85	0.40
1:B:360:ALA:CB	1:B:365:THR:HG22	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	320/336 (95%)	284 (89%)	31 (10%)	5 (2%)	9	37
1	C	322/336 (96%)	300 (93%)	19 (6%)	3 (1%)	17	51
2	A	1024/1054 (97%)	923 (90%)	91 (9%)	10 (1%)	15	48
All	All	1666/1726 (96%)	1507 (90%)	141 (8%)	18 (1%)	14	46

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	ALA
2	A	638	PRO
2	A	852	PRO
1	B	292	ARG
1	C	172	GLY
1	B	390	ASN
2	A	574	PRO
2	A	813	LEU
1	B	388	GLU
2	A	56	GLN
2	A	812	MET
2	A	998	ILE
2	A	1024	PRO
2	A	665	PRO
1	B	137	PRO
1	C	137	PRO
1	B	156	PRO
2	A	426	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	B	263/275 (96%)	235 (89%)	28 (11%)	6	25
1	C	265/275 (96%)	236 (89%)	29 (11%)	6	24
2	A	847/871 (97%)	762 (90%)	85 (10%)	7	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1375/1421 (97%)	1233 (90%)	142 (10%)	7 27

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	105	THR
1	B	117	ASN
1	B	121	TYR
1	B	151	LEU
1	B	206	THR
1	B	239	GLN
1	B	247	THR
1	B	266	LEU
1	B	267	THR
1	B	268	VAL
1	B	275	THR
1	B	276	LEU
1	B	280	LYS
1	B	282	THR
1	B	298	LEU
1	B	322	GLU
1	B	332	LEU
1	B	335	THR
1	B	340	ARG
1	B	349	ARG
1	B	351	VAL
1	B	357	VAL
1	B	364	VAL
1	B	378	VAL
1	B	390	ASN
1	B	395	LEU
1	B	396	GLU
1	C	87	THR
1	C	96	THR
1	C	104	LEU
1	C	120	GLN
1	C	121	TYR
1	C	150	LEU
1	C	151	LEU
1	C	185	LEU
1	C	207	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	247	THR
1	C	253	SER
1	C	257	LEU
1	C	260	ASP
1	C	268	VAL
1	C	283	LEU
1	C	287	VAL
1	C	292	ARG
1	C	304	ASP
1	C	316	GLN
1	C	317	LEU
1	C	324	MET
1	C	325	LEU
1	C	330	GLN
1	C	339	GLN
1	C	354	ARG
1	C	364	VAL
1	C	365	THR
1	C	367	LEU
1	C	382	LEU
2	A	6	ILE
2	A	8	ARG
2	A	34	THR
2	A	42	LEU
2	A	48	ILE
2	A	51	THR
2	A	53	TYR
2	A	65	VAL
2	A	88	PHE
2	A	105	TRP
2	A	114	LEU
2	A	140	TYR
2	A	145	VAL
2	A	157	ARG
2	A	184	VAL
2	A	203	LEU
2	A	211	ASP
2	A	215	GLN
2	A	236	TYR
2	A	259	LEU
2	A	260	ARG
2	A	298	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	338	LEU
2	A	343	LEU
2	A	374	LEU
2	A	403	MET
2	A	412	GLU
2	A	418	LEU
2	A	434	THR
2	A	436	TRP
2	A	464	ILE
2	A	492	LEU
2	A	521	LEU
2	A	524	VAL
2	A	531	LYS
2	A	532	VAL
2	A	534	HIS
2	A	541	LEU
2	A	545	LEU
2	A	547	VAL
2	A	567	GLU
2	A	569	ASP
2	A	573	MET
2	A	602	VAL
2	A	623	MET
2	A	624	VAL
2	A	634	GLU
2	A	637	ARG
2	A	642	MET
2	A	643	ASP
2	A	660	ASN
2	A	661	LEU
2	A	663	VAL
2	A	688	THR
2	A	693	ILE
2	A	722	ARG
2	A	725	ASN
2	A	729	ASN
2	A	748	THR
2	A	769	ASN
2	A	771	ARG
2	A	778	ASP
2	A	781	GLN
2	A	786	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	789	LEU
2	A	804	ILE
2	A	812	MET
2	A	813	LEU
2	A	884	PHE
2	A	885	VAL
2	A	888	TYR
2	A	899	LEU
2	A	904	VAL
2	A	909	VAL
2	A	945	LEU
2	A	946	MET
2	A	955	VAL
2	A	958	LEU
2	A	969	LEU
2	A	970	ASP
2	A	984	LYS
2	A	999	LEU
2	A	1020	MET
2	A	1035	TYR
2	A	1039	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	120	GLN
1	B	125	GLN
1	B	177	GLN
1	B	295	GLN
1	B	302	ASN
1	B	330	GLN
1	B	390	ASN
1	C	125	GLN
1	C	177	GLN
1	C	295	GLN
1	C	302	ASN
2	A	87	GLN
2	A	118	GLN
2	A	151	HIS
2	A	215	GLN
2	A	238	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	279	ASN
2	A	329	GLN
2	A	359	HIS
2	A	413	ASN
2	A	423	HIS
2	A	470	GLN
2	A	534	HIS
2	A	564	GLN
2	A	590	GLN
2	A	629	GLN
2	A	633	GLN
2	A	635	GLN
2	A	660	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS
2	A	921	HIS
2	A	1043	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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	B	322/336 (95%)	-0.06	3 (0%) 84 88	24, 58, 112, 176	0
1	C	324/336 (96%)	-0.01	2 (0%) 89 92	25, 58, 110, 174	0
2	A	1028/1054 (97%)	0.40	107 (10%) 6 8	28, 106, 212, 312	0
All	All	1674/1726 (96%)	0.23	112 (6%) 17 21	24, 79, 194, 312	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	15	LEU	10.7
2	A	890	ALA	8.4
2	A	365	VAL	7.7
2	A	887	LEU	7.7
2	A	495	VAL	5.8
2	A	889	LEU	5.4
2	A	886	LEU	5.1
2	A	494	ILE	5.0
2	A	496	VAL	4.9
2	A	891	PHE	4.9
2	A	418	LEU	4.8
2	A	1036	LYS	4.7
2	A	368	ILE	4.7
2	A	888	TYR	4.6
2	A	429	THR	4.6
2	A	17	LEU	4.6
2	A	18	MET	4.5
2	A	873	LYS	4.4
2	A	436	TRP	4.4
1	C	402	SER	4.3
2	A	73	MET	4.2
2	A	872	LEU	4.2
2	A	14	PHE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	499	ILE	4.2
2	A	853	GLY	4.1
2	A	7	ARG	4.1
2	A	355	LEU	4.1
2	A	538	THR	4.0
2	A	848	VAL	3.9
2	A	1001	GLY	3.8
2	A	449	ALA	3.8
2	A	1043	HIS	3.7
2	A	29	TRP	3.7
2	A	428	ALA	3.7
2	A	504	TRP	3.6
2	A	437	GLN	3.6
2	A	35	PRO	3.6
2	A	704	ALA	3.5
2	A	1035	TYR	3.5
2	A	1039	TRP	3.5
2	A	445	GLU	3.5
2	A	528	LEU	3.4
2	A	874	LEU	3.4
2	A	502	GLY	3.4
2	A	847	LYS	3.3
2	A	392	SER	3.3
2	A	703	VAL	3.2
2	A	423	HIS	3.2
2	A	500	LEU	3.2
2	A	427	ASP	3.1
2	A	450	LEU	3.1
2	A	396	ILE	3.0
2	A	71	THR	3.0
2	A	451	PHE	3.0
2	A	434	THR	2.9
2	A	554	LEU	2.9
2	A	426	PRO	2.9
2	A	539	THR	2.9
2	A	430	LEU	2.9
2	A	498	PRO	2.9
2	A	530	LEU	2.7
2	A	16	VAL	2.7
2	A	417	ARG	2.7
2	A	366	ALA	2.6
2	A	895	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	896	GLU	2.6
2	A	956	PRO	2.5
2	A	36	VAL	2.5
2	A	439	ILE	2.5
2	A	871	LYS	2.5
2	A	946	MET	2.5
2	A	421	TRP	2.5
2	A	497	ILE	2.5
2	A	26	TRP	2.4
2	A	1037	LEU	2.4
1	B	79	ALA	2.4
1	B	387	SER	2.4
2	A	438	VAL	2.4
2	A	846	GLU	2.4
2	A	1041	HIS	2.4
2	A	875	MET	2.4
2	A	448	PRO	2.4
2	A	970	ASP	2.3
2	A	669	ARG	2.3
1	B	386	ASP	2.3
2	A	700	ILE	2.3
2	A	480	PHE	2.3
2	A	462	ILE	2.3
2	A	388	ALA	2.3
2	A	503	TYR	2.3
2	A	120	LYS	2.2
2	A	948	LEU	2.2
2	A	520	PHE	2.2
2	A	849	GLN	2.2
2	A	32	ILE	2.2
2	A	960	ASN	2.2
2	A	954	ALA	2.2
2	A	623	MET	2.2
2	A	549	THR	2.1
2	A	973	LEU	2.1
2	A	78	GLY	2.1
2	A	11	ALA	2.1
2	A	850	LEU	2.1
2	A	33	ASN	2.1
1	C	242	ASP	2.1
2	A	854	THR	2.1
2	A	517	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	433	LYS	2.1
2	A	441	ASP	2.1
2	A	406	ALA	2.0
2	A	969	LEU	2.0
2	A	10	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CU	A	1048	1/1	0.92	0.19	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.