



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

PDB ID : 3UU0
Title : Crystal structure of L-rhamnose isomerase from *Bacillus halodurans* in complex with Mn
Authors : Doan, T.T.N.; Prabhu, P.; Kim, J.K.; Jeya, M.; Kang, L.W.; Lee, J.K.
Deposited on : 2011-11-27
Resolution : 2.70 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

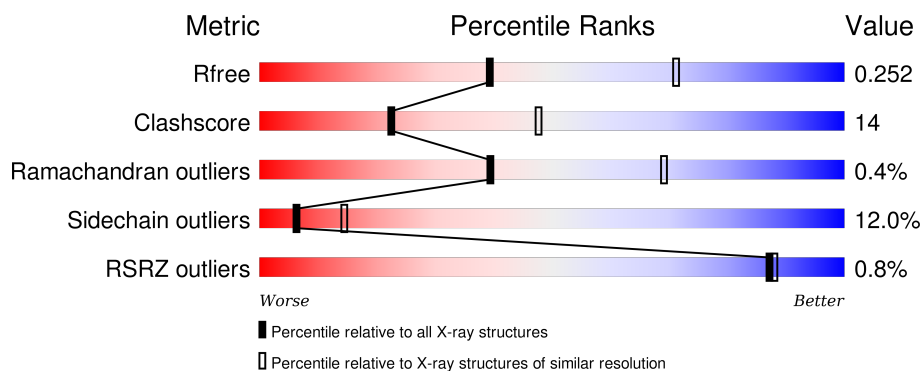
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	424	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>5%</div> <div>5%</div> </div> </div>
1	B	424	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>•</div> <div>5%</div> </div> </div>
1	C	424	<div> <div></div> <div> <div></div> <div>69%</div> <div>21%</div> <div>5%</div> <div>5%</div> </div> </div>
1	D	424	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>•</div> <div>5%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	B	420	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13491 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 L-rhamnose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3286	2107	565	605	9			
1	B	402	Total	C	N	O	S	0	0	0
			3290	2109	566	606	9			
1	C	403	Total	C	N	O	S	0	0	0
			3296	2112	567	608	9			
1	D	404	Total	C	N	O	S	0	0	0
			3304	2117	568	609	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	C	2	Total 2	Mn 2	0	0

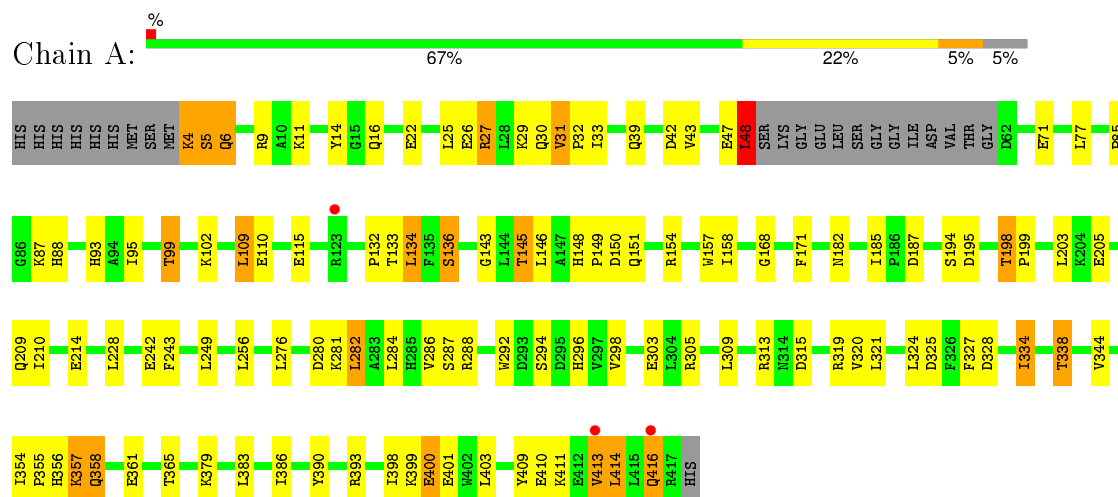
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total 78	O 78	0	0
3	B	83	Total 83	O 83	0	0
3	C	73	Total 73	O 73	0	0
3	D	73	Total 73	O 73	0	0

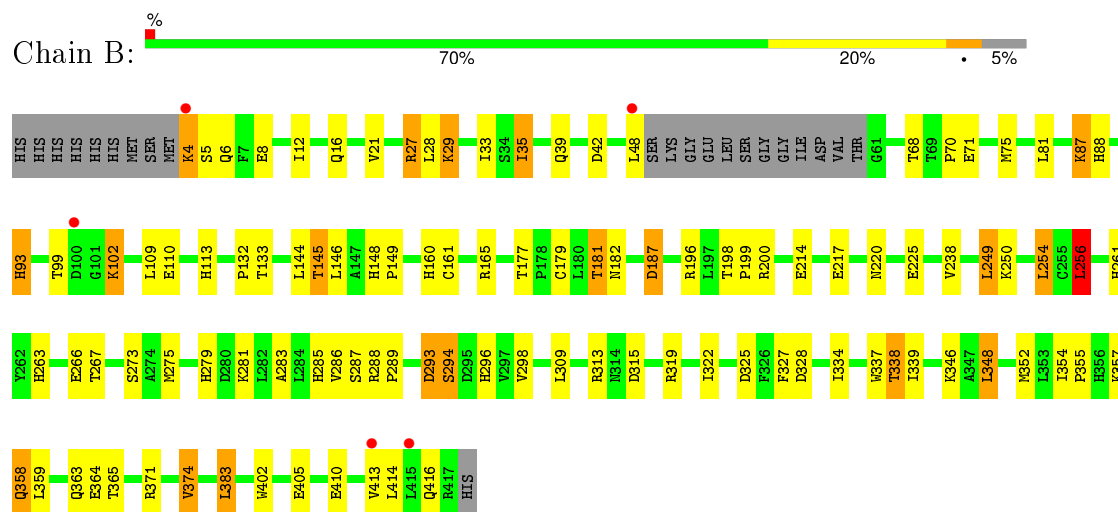
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

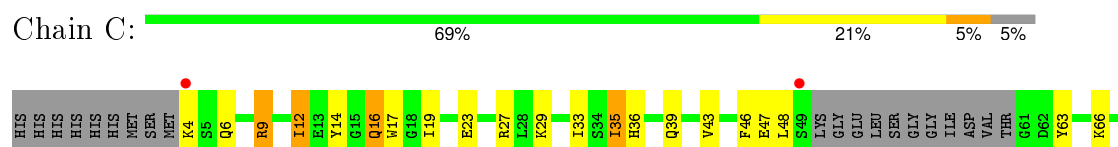
• Molecule 1: L-rhamnose isomerase

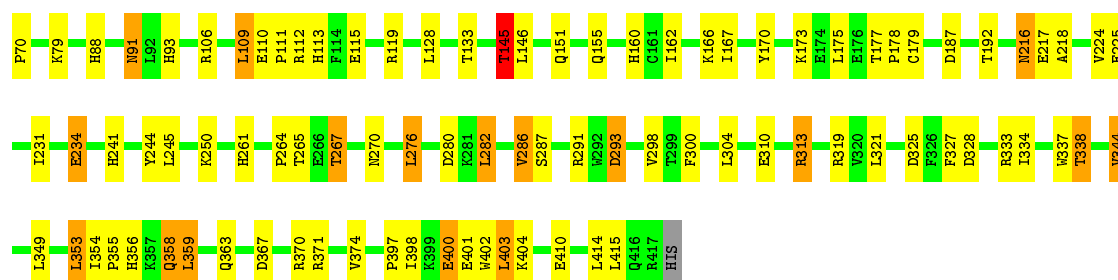


• Molecule 1: L-rhamnose isomerase

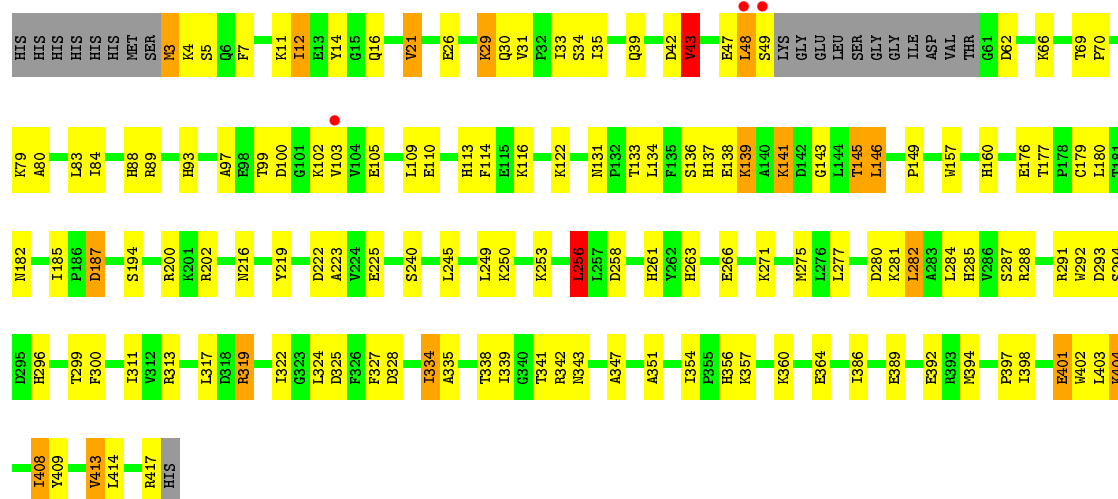


• Molecule 1: L-rhamnose isomerase





• Molecule 1: L-rhamnose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.58Å 165.55Å 92.47Å 90.00° 115.82° 90.00°	Depositor
Resolution (Å)	46.62 – 2.70 46.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.62-2.70) 96.0 (46.62-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.255 0.183 , 0.252	Depositor DCC
R_{free} test set	3022 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59483 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13491	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.88	1/3367 (0.0%)	0.87	4/4559 (0.1%)
1	B	0.91	1/3371 (0.0%)	0.89	4/4564 (0.1%)
1	C	0.88	2/3377 (0.1%)	0.88	2/4572 (0.0%)
1	D	0.87	1/3385 (0.0%)	0.88	4/4582 (0.1%)
All	All	0.89	5/13500 (0.0%)	0.88	14/18277 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	GLU	CD-OE1	-5.71	1.19	1.25
1	C	63	TYR	CE2-CZ	-5.52	1.31	1.38
1	C	63	TYR	CD2-CE2	-5.44	1.31	1.39
1	D	225	GLU	CD-OE1	-5.41	1.19	1.25
1	A	214	GLU	CG-CD	5.33	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	293	ASP	CB-CG-OD1	7.29	124.86	118.30
1	D	256	LEU	CA-CB-CG	6.39	130.01	115.30
1	B	254	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	48	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	134	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	256	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	334	ILE	CG1-CB-CG2	-5.66	98.95	111.40
1	D	284	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	29	LYS	CD-CE-NZ	5.51	124.37	111.70
1	D	293	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	282	LEU	CB-CG-CD1	-5.14	102.27	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	ARG	CB-CA-C	-5.11	100.17	110.40
1	D	324	LEU	C-N-CA	-5.10	108.96	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3286	0	3241	90	0
1	B	3290	0	3244	84	0
1	C	3296	0	3249	83	0
1	D	3304	0	3258	112	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	78	0	0	1	0
3	B	83	0	0	2	0
3	C	73	0	0	0	0
3	D	73	0	0	5	0
All	All	13491	0	12992	359	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 14.

All (359) 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:D:48:LEU:HD22	1:D:49:SER:N	1.53	1.19
1:D:145:THR:CG2	1:D:146:LEU:H	1.60	1.13
1:D:48:LEU:HG	1:D:103:VAL:HG12	1.24	1.12
1:B:145:THR:HG22	1:B:146:LEU:H	1.00	1.11
1:C:286:VAL:HG23	1:C:298:VAL:HG21	1.33	1.09
1:B:4:LYS:HD3	1:B:4:LYS:N	1.68	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:THR:HG22	1:D:146:LEU:H	1.22	1.04
1:B:145:THR:HG22	1:B:146:LEU:N	1.67	1.04
1:A:145:THR:HG22	1:A:146:LEU:H	1.22	1.02
1:C:264:PRO:O	1:C:265:THR:HB	1.54	1.01
1:A:4:LYS:HG2	1:A:6:GLN:HB3	1.42	1.00
1:D:48:LEU:C	1:D:48:LEU:CD2	2.30	0.99
1:C:145:THR:CG2	1:C:146:LEU:H	1.79	0.95
1:D:145:THR:CG2	1:D:146:LEU:N	2.29	0.94
1:D:48:LEU:CD2	1:D:49:SER:N	2.30	0.94
1:A:4:LYS:CG	1:A:6:GLN:HB3	1.98	0.93
1:B:110:GLU:H	1:B:113:HIS:HD2	1.09	0.92
1:B:133:THR:H	1:B:160:HIS:HE1	1.15	0.91
1:A:4:LYS:HG3	1:A:6:GLN:H	1.36	0.91
1:A:145:THR:HG22	1:A:146:LEU:N	1.88	0.89
1:C:145:THR:HG22	1:C:146:LEU:H	1.36	0.88
1:D:48:LEU:HD13	1:D:48:LEU:H	1.39	0.88
1:B:145:THR:CG2	1:B:146:LEU:H	1.88	0.86
1:B:334:ILE:O	1:B:338:THR:HG23	1.76	0.86
1:D:48:LEU:CG	1:D:103:VAL:HG12	2.05	0.85
1:A:357:LYS:CD	1:A:357:LYS:H	1.84	0.84
1:A:357:LYS:H	1:A:357:LYS:HD3	1.42	0.84
1:B:200:ARG:HD2	1:B:238:VAL:O	1.77	0.84
1:A:148:HIS:HD2	1:A:150:ASP:H	1.22	0.84
1:D:48:LEU:C	1:D:48:LEU:HD22	1.88	0.84
1:D:133:THR:H	1:D:160:HIS:HE1	1.26	0.83
1:C:358:GLN:HE21	1:C:358:GLN:H	1.27	0.82
1:D:145:THR:HG23	1:D:146:LEU:H	1.45	0.81
1:B:145:THR:CG2	1:B:146:LEU:N	2.39	0.81
1:B:87:LYS:HE2	1:B:87:LYS:CA	2.07	0.81
1:A:195:ASP:OD2	1:A:198:THR:HG23	1.80	0.80
1:A:286:VAL:HG23	1:A:298:VAL:HG21	1.63	0.80
1:D:48:LEU:HD23	1:D:49:SER:OG	1.80	0.80
1:D:48:LEU:HG	1:D:103:VAL:CG1	2.10	0.79
1:D:14:TYR:CE2	1:D:386:ILE:CD1	2.65	0.79
1:A:358:GLN:H	1:A:358:GLN:HE21	1.29	0.79
1:D:334:ILE:O	1:D:338:THR:HG23	1.83	0.78
1:B:286:VAL:HG23	1:B:298:VAL:HG21	1.67	0.77
1:D:335:ALA:O	1:D:339:ILE:HG13	1.83	0.77
1:C:145:THR:CG2	1:C:146:LEU:N	2.48	0.77
1:C:35:ILE:HD12	1:C:337:TRP:CD1	2.19	0.76
1:A:99:THR:CG2	1:A:102:LYS:O	2.33	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:HB	1:B:187:ASP:OD1	1.85	0.75
1:A:357:LYS:HG2	1:A:358:GLN:NE2	2.02	0.75
1:D:145:THR:HG23	1:D:146:LEU:N	1.97	0.74
1:B:181:THR:HG23	1:B:220:ASN:OD1	1.87	0.74
1:D:145:THR:HG22	1:D:146:LEU:N	2.00	0.73
1:B:93:HIS:HD2	1:B:133:THR:OG1	1.72	0.72
1:C:310:GLU:OE2	1:C:313:ARG:NH1	2.22	0.72
1:D:48:LEU:HD22	1:D:49:SER:H	1.53	0.72
1:A:145:THR:CG2	1:A:146:LEU:N	2.52	0.71
1:A:134:LEU:HG	1:A:185:ILE:HG22	1.71	0.71
1:C:110:GLU:H	1:C:113:HIS:HD2	1.39	0.71
1:B:133:THR:H	1:B:160:HIS:CE1	2.05	0.71
1:D:48:LEU:C	1:D:48:LEU:HD23	2.10	0.70
1:D:39:GLN:HE22	1:D:328:ASP:H	1.40	0.70
1:D:39:GLN:NE2	1:D:327:PHE:HA	2.07	0.69
1:B:287:SER:HB3	1:B:325:ASP:O	1.92	0.69
1:A:286:VAL:CG2	1:A:298:VAL:HG21	2.22	0.69
1:B:4:LYS:CD	1:B:4:LYS:N	2.45	0.68
1:B:110:GLU:N	1:B:113:HIS:HD2	1.86	0.68
1:A:47:GLU:O	1:A:48:LEU:C	2.33	0.68
1:B:363:GLN:HE21	1:B:371:ARG:HH11	1.41	0.68
1:D:417:ARG:HH11	1:D:417:ARG:HB3	1.58	0.68
1:A:4:LYS:HG3	1:A:6:GLN:N	2.07	0.67
1:B:87:LYS:HE2	1:B:87:LYS:HA	1.74	0.67
1:C:287:SER:HB3	1:C:325:ASP:O	1.94	0.67
1:B:359:LEU:HD21	1:B:374:VAL:HG22	1.75	0.67
1:A:334:ILE:O	1:A:338:THR:HG23	1.95	0.67
1:D:14:TYR:CE2	1:D:386:ILE:HD11	2.29	0.67
1:D:110:GLU:H	1:D:113:HIS:HD2	1.41	0.67
1:B:256:LEU:HD22	1:B:283:ALA:CB	2.25	0.67
1:B:256:LEU:HD22	1:B:283:ALA:HB1	1.78	0.67
1:D:48:LEU:CD2	1:D:49:SER:CB	2.74	0.66
1:A:286:VAL:HG23	1:A:298:VAL:CG2	2.25	0.65
1:D:417:ARG:HB3	1:D:417:ARG:NH1	2.12	0.65
1:C:216:ASN:HD22	1:C:217:GLU:N	1.94	0.65
1:B:363:GLN:HE22	1:D:194:SER:H	1.42	0.65
1:A:303:GLU:HA	1:A:303:GLU:OE1	1.97	0.65
1:C:286:VAL:HG23	1:C:298:VAL:CG2	2.19	0.65
1:B:110:GLU:H	1:B:113:HIS:CD2	2.02	0.65
1:D:351:ALA:O	1:D:356:HIS:HE1	1.80	0.65
1:B:133:THR:N	1:B:160:HIS:HE1	1.92	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:HIS:CD2	1:A:150:ASP:H	2.11	0.64
1:C:217:GLU:H	1:C:217:GLU:CD	2.01	0.64
1:A:194:SER:H	1:C:363:GLN:NE2	1.94	0.64
1:A:357:LYS:N	1:A:357:LYS:HD3	2.12	0.64
1:D:356:HIS:O	1:D:360:LYS:HG3	1.97	0.64
1:A:194:SER:H	1:C:363:GLN:HE22	1.46	0.64
1:B:256:LEU:HD11	1:B:285:HIS:CG	2.33	0.63
1:A:410:GLU:HA	1:A:414:LEU:HB2	1.80	0.63
1:A:357:LYS:HG2	1:A:358:GLN:HE21	1.63	0.63
1:C:334:ILE:O	1:C:338:THR:HG22	1.99	0.63
1:D:79:LYS:HD2	1:D:409:TYR:CD1	2.34	0.63
1:B:294:SER:HB2	1:B:296:HIS:ND1	2.13	0.63
1:C:267:THR:HG22	1:C:270:ASN:HB3	1.80	0.63
1:C:128:LEU:HD22	1:C:175:LEU:HD11	1.81	0.62
1:D:182:ASN:HD22	1:D:223:ALA:HB3	1.63	0.62
1:B:249:LEU:HD22	1:B:279:HIS:CE1	2.35	0.62
1:C:112:ARG:HG2	1:C:112:ARG:HH11	1.65	0.62
1:C:355:PRO:HG2	1:C:359:LEU:HD22	1.82	0.61
1:D:397:PRO:HB3	1:D:401:GLU:HB3	1.81	0.61
1:D:48:LEU:CD1	1:D:48:LEU:H	2.09	0.61
1:A:145:THR:HB	1:A:187:ASP:OD1	2.00	0.61
1:D:275:MET:CB	1:D:282:LEU:HD11	2.31	0.60
1:A:134:LEU:HD13	1:A:157:TRP:CE3	2.36	0.60
1:A:416:GLN:C	1:A:416:GLN:HE21	2.03	0.60
1:C:106:ARG:HA	1:C:109:LEU:CD2	2.32	0.60
1:A:356:HIS:N	1:A:357:LYS:HE3	2.17	0.60
1:C:115:GLU:OE2	1:C:119:ARG:NH2	2.34	0.60
1:D:3:MET:O	1:D:3:MET:HG3	1.99	0.60
1:C:334:ILE:HD13	1:C:414:LEU:HD11	1.82	0.60
1:A:99:THR:HG21	1:A:102:LYS:O	2.00	0.60
1:C:110:GLU:H	1:C:113:HIS:CD2	2.19	0.60
1:A:358:GLN:NE2	1:A:358:GLN:H	1.99	0.59
1:C:267:THR:HG23	1:C:270:ASN:H	1.66	0.59
1:A:416:GLN:O	1:A:416:GLN:NE2	2.30	0.59
1:C:363:GLN:HE21	1:C:371:ARG:HH11	1.47	0.59
1:D:39:GLN:HE22	1:D:327:PHE:HA	1.67	0.58
1:B:266:GLU:HG3	1:D:263:HIS:CE1	2.38	0.58
1:C:106:ARG:HA	1:C:109:LEU:HD22	1.85	0.58
1:A:25:LEU:HD22	1:A:390:TYR:HD1	1.67	0.58
1:D:48:LEU:CD2	1:D:49:SER:OG	2.51	0.57
1:A:26:GLU:O	1:A:30:GLN:HG2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:HA	1:C:115:GLU:HG3	1.87	0.57
1:D:180:LEU:HD11	1:D:223:ALA:HB2	1.85	0.57
1:A:288:ARG:HD2	3:A:439:HOH:O	2.05	0.57
1:D:133:THR:N	1:D:160:HIS:HE1	1.99	0.56
1:B:334:ILE:O	1:B:338:THR:CG2	2.51	0.56
1:B:363:GLN:NE2	1:D:194:SER:H	2.04	0.56
1:B:273:SER:HB2	1:D:200:ARG:HH11	1.71	0.56
1:A:99:THR:HG23	1:A:99:THR:O	2.05	0.56
1:D:83:LEU:HD22	1:D:402:TRP:HB2	1.88	0.56
1:A:25:LEU:HD22	1:A:390:TYR:CD1	2.41	0.56
1:C:17:TRP:HB2	1:C:19:ILE:HG12	1.88	0.56
1:C:167:ILE:O	1:C:170:TYR:HB3	2.06	0.56
1:C:264:PRO:O	1:C:265:THR:CB	2.36	0.56
1:B:363:GLN:NE2	1:B:371:ARG:HH11	2.03	0.56
1:B:93:HIS:CD2	1:B:133:THR:OG1	2.58	0.56
1:D:134:LEU:HD13	1:D:185:ILE:HG22	1.87	0.55
1:B:263:HIS:CE1	1:D:266:GLU:HA	2.42	0.55
1:B:39:GLN:HE22	1:B:328:ASP:H	1.52	0.55
1:D:325:ASP:OD1	3:D:478:HOH:O	2.18	0.55
1:B:42:ASP:HA	1:B:327:PHE:CE1	2.41	0.55
1:A:305:ARG:O	1:A:309:LEU:HG	2.06	0.55
1:D:275:MET:HB2	1:D:282:LEU:HD11	1.88	0.55
1:B:12:ILE:O	1:B:16:GLN:HG3	2.06	0.55
1:D:413:VAL:HG23	1:D:414:LEU:N	2.22	0.55
1:D:12:ILE:O	1:D:16:GLN:HG3	2.07	0.54
1:C:145:THR:HG23	1:C:146:LEU:H	1.67	0.54
1:D:413:VAL:HG23	1:D:414:LEU:H	1.73	0.54
1:B:364:GLU:OE2	1:D:202:ARG:NH2	2.41	0.54
1:B:198:THR:HB	1:B:199:PRO:HD3	1.89	0.54
1:D:14:TYR:CD2	1:D:386:ILE:HD11	2.42	0.54
1:C:133:THR:H	1:C:160:HIS:HE1	1.54	0.54
1:A:39:GLN:HE22	1:A:328:ASP:H	1.55	0.54
1:B:354:ILE:HG23	1:B:355:PRO:HD2	1.89	0.54
1:B:8:GLU:OE1	1:B:8:GLU:HA	2.07	0.54
1:D:133:THR:H	1:D:160:HIS:CE1	2.16	0.54
1:A:280:ASP:O	1:A:319:ARG:HD2	2.08	0.54
1:D:99:THR:O	1:D:100:ASP:HB2	2.08	0.54
1:D:256:LEU:HD11	1:D:285:HIS:CG	2.44	0.53
1:A:99:THR:CG2	1:A:99:THR:O	2.56	0.53
1:B:161:CYS:O	1:B:165:ARG:HG3	2.08	0.53
1:C:358:GLN:NE2	1:C:358:GLN:H	2.03	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:CG2	1:B:220:ASN:OD1	2.55	0.53
1:D:300:PHE:HE1	1:D:347:ALA:HA	1.72	0.53
1:A:409:TYR:CE1	1:A:413:VAL:HG21	2.44	0.53
1:C:402:TRP:CZ3	1:C:403:LEU:HD13	2.43	0.53
1:A:6:GLN:HA	1:A:6:GLN:HE21	1.74	0.53
1:C:112:ARG:HG2	1:C:112:ARG:NH1	2.23	0.52
1:A:398:ILE:O	1:A:401:GLU:HG2	2.09	0.52
1:B:179:CYS:SG	1:B:181:THR:HG22	2.50	0.52
1:D:413:VAL:CG2	1:D:414:LEU:N	2.73	0.52
1:A:4:LYS:CG	1:A:6:GLN:CB	2.83	0.52
1:C:145:THR:HG23	1:C:146:LEU:N	2.24	0.52
1:D:14:TYR:HE2	1:D:386:ILE:CD1	2.17	0.52
1:B:364:GLU:OE2	1:D:149:PRO:HB3	2.10	0.52
1:A:132:PRO:HD2	1:A:182:ASN:O	2.09	0.52
1:D:143:GLY:O	1:D:187:ASP:HA	2.10	0.52
1:A:4:LYS:HG3	1:A:6:GLN:HB3	1.88	0.52
1:C:110:GLU:N	1:C:113:HIS:HD2	2.04	0.52
1:C:286:VAL:CG2	1:C:298:VAL:HG21	2.23	0.52
1:B:196:ARG:NH2	3:B:484:HOH:O	2.30	0.52
1:B:261:HIS:CD2	1:B:293:ASP:OD2	2.63	0.52
1:C:224:VAL:HB	1:C:244:TYR:CD1	2.45	0.52
1:D:7:PHE:CE1	1:D:389:GLU:HG2	2.44	0.51
1:D:69:THR:HB	1:D:70:PRO:HD2	1.92	0.51
1:D:29:LYS:HB3	1:D:394:MET:HE3	1.93	0.51
1:C:39:GLN:HE22	1:C:328:ASP:H	1.58	0.51
1:C:367:ASP:OD2	1:C:370:ARG:HD2	2.11	0.51
1:D:48:LEU:CB	1:D:103:VAL:HG12	2.40	0.51
1:C:35:ILE:CD1	1:C:337:TRP:CD1	2.92	0.51
1:D:258:ASP:HB3	1:D:261:HIS:CG	2.46	0.51
1:A:148:HIS:CD2	1:A:149:PRO:HD2	2.46	0.51
1:C:216:ASN:HD22	1:C:217:GLU:H	1.58	0.51
1:D:83:LEU:O	1:D:342:ARG:NH1	2.43	0.51
1:B:256:LEU:CD2	1:B:283:ALA:HB1	2.41	0.51
1:C:12:ILE:O	1:C:16:GLN:HG2	2.10	0.51
1:D:311:ILE:HG22	1:D:317:LEU:HD23	1.93	0.51
1:C:370:ARG:O	1:C:374:VAL:HG13	2.11	0.50
1:B:35:ILE:HD12	1:B:337:TRP:CD1	2.46	0.50
1:A:398:ILE:HG13	1:A:399:LYS:HG3	1.92	0.50
1:D:311:ILE:HD13	1:D:322:ILE:HD11	1.93	0.50
1:D:26:GLU:O	1:D:29:LYS:HG3	2.11	0.50
1:D:3:MET:HG3	1:D:4:LYS:CD	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ARG:NH2	3:B:458:HOH:O	2.44	0.50
1:C:333:ARG:HG3	1:C:333:ARG:HH11	1.78	0.49
1:D:275:MET:HB3	1:D:282:LEU:HD11	1.95	0.49
1:B:339:ILE:HG13	1:B:402:TRP:CH2	2.47	0.49
1:D:3:MET:HG3	1:D:4:LYS:HD2	1.94	0.48
1:B:263:HIS:HE1	3:D:431:HOH:O	1.97	0.48
1:A:95:ILE:HG23	1:A:133:THR:HG21	1.95	0.48
1:B:355:PRO:HB2	1:B:358:GLN:HG3	1.95	0.48
1:D:311:ILE:CG2	1:D:317:LEU:HD23	2.43	0.48
1:C:66:LYS:HB3	1:C:333:ARG:CZ	2.43	0.48
1:B:287:SER:CB	1:B:325:ASP:O	2.59	0.48
1:D:404:LYS:NZ	1:D:404:LYS:HA	2.28	0.48
1:D:48:LEU:HD23	1:D:49:SER:CB	2.43	0.47
1:B:348:LEU:O	1:B:352:MET:HG3	2.14	0.47
1:B:148:HIS:ND1	1:B:149:PRO:HD2	2.29	0.47
1:A:413:VAL:O	1:A:414:LEU:C	2.52	0.47
1:A:27:ARG:HD2	1:A:27:ARG:HA	1.33	0.47
1:D:292:TRP:O	1:D:294:SER:N	2.45	0.47
1:D:280:ASP:O	1:D:319:ARG:HD2	2.14	0.47
1:A:148:HIS:O	1:A:154:ARG:HD3	2.15	0.47
1:D:110:GLU:H	1:D:113:HIS:CD2	2.28	0.47
1:B:102:LYS:HG3	1:B:102:LYS:H	1.45	0.47
1:C:261:HIS:CD2	1:C:293:ASP:OD2	2.67	0.46
1:B:410:GLU:HA	1:B:414:LEU:HB2	1.97	0.46
1:C:349:LEU:O	1:C:353:LEU:HD22	2.15	0.46
1:D:11:LYS:HG3	1:D:21:VAL:HG22	1.96	0.46
1:C:400:GLU:O	1:C:403:LEU:HB2	2.15	0.46
1:C:397:PRO:HB3	1:C:401:GLU:HB2	1.96	0.46
1:D:39:GLN:HE22	1:D:328:ASP:N	2.10	0.46
1:D:34:SER:HA	1:D:89:ARG:HB2	1.98	0.46
1:D:200:ARG:NH2	1:D:240:SER:HB3	2.30	0.46
1:D:222:ASP:HB2	1:D:253:LYS:HD2	1.98	0.46
1:B:4:LYS:HG2	1:B:6:GLN:HG3	1.97	0.46
1:A:195:ASP:OD2	1:A:198:THR:CG2	2.60	0.46
1:C:128:LEU:HB2	1:C:175:LEU:CD1	2.46	0.46
1:C:9:ARG:HA	1:C:12:ILE:HD13	1.98	0.46
1:D:288:ARG:HB3	1:D:296:HIS:HB2	1.97	0.46
1:D:216:ASN:HB3	1:D:219:TYR:CD2	2.51	0.46
1:D:138:GLU:O	1:D:141:LYS:HD2	2.15	0.46
1:B:99:THR:HG21	1:B:102:LYS:O	2.15	0.45
1:C:14:TYR:HB3	1:C:19:ILE:HB	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:O	1:B:88:HIS:HB3	2.16	0.45
1:B:383:LEU:O	1:B:383:LEU:HD22	2.16	0.45
1:D:131:ASN:ND2	1:D:182:ASN:HB3	2.31	0.45
1:D:398:ILE:O	1:D:401:GLU:HB2	2.17	0.45
1:D:287:SER:HB3	1:D:325:ASP:O	2.16	0.45
1:A:356:HIS:H	1:A:357:LYS:HE3	1.82	0.45
1:B:413:VAL:HG23	1:B:414:LEU:HD23	1.99	0.45
1:A:85:PRO:O	1:A:88:HIS:HE1	1.99	0.45
1:C:276:LEU:HD13	1:C:282:LEU:HD21	1.99	0.45
1:A:357:LYS:CG	1:A:358:GLN:NE2	2.76	0.44
1:B:359:LEU:HD21	1:B:374:VAL:CG2	2.46	0.44
1:A:14:TYR:CE2	1:A:386:ILE:CD1	3.00	0.44
1:C:410:GLU:HA	1:C:414:LEU:HB2	2.00	0.44
1:A:33:ILE:O	1:A:88:HIS:HB3	2.17	0.44
1:A:294:SER:OG	1:A:296:HIS:CD2	2.70	0.44
1:A:185:ILE:HD12	1:A:187:ASP:CG	2.38	0.44
1:A:22:GLU:CD	1:A:393:ARG:HH12	2.21	0.44
1:D:84:ILE:HG21	1:D:341:THR:HG21	2.00	0.44
1:C:110:GLU:HG2	1:C:111:PRO:HD2	1.99	0.44
1:B:263:HIS:CE1	3:D:431:HOH:O	2.71	0.44
1:C:398:ILE:O	1:C:401:GLU:HG2	2.17	0.44
1:B:256:LEU:HD11	1:B:285:HIS:ND1	2.32	0.44
1:C:133:THR:N	1:C:160:HIS:HE1	2.16	0.44
1:D:299:THR:HA	1:D:343:ASN:ND2	2.33	0.44
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.80	0.44
1:A:282:LEU:HD23	1:A:320:VAL:HG22	1.99	0.44
1:B:263:HIS:HD2	1:B:266:GLU:OE1	2.01	0.44
1:A:158:ILE:HG23	1:A:210:ILE:HG13	2.00	0.44
1:A:198:THR:N	1:A:199:PRO:HD2	2.32	0.43
1:A:182:ASN:ND2	1:A:256:LEU:HD13	2.32	0.43
1:C:415:LEU:HA	1:C:415:LEU:HD23	1.66	0.43
1:C:265:THR:HG22	1:C:265:THR:O	2.18	0.43
1:C:46:PHE:CZ	1:C:70:PRO:HA	2.53	0.43
1:A:42:ASP:HA	1:A:327:PHE:CE2	2.53	0.43
1:B:256:LEU:HD22	1:B:283:ALA:HB3	1.99	0.43
1:D:100:ASP:OD2	3:D:440:HOH:O	2.21	0.43
1:B:99:THR:CG2	1:B:102:LYS:O	2.67	0.43
1:B:309:LEU:O	1:B:313:ARG:HB2	2.18	0.43
1:C:216:ASN:ND2	1:C:218:ALA:H	2.17	0.43
1:B:294:SER:HB2	1:B:296:HIS:CE1	2.54	0.43
1:B:198:THR:N	1:B:199:PRO:CD	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLU:OE2	1:C:241:HIS:HE1	2.01	0.43
1:D:33:ILE:O	1:D:88:HIS:HB3	2.18	0.43
1:C:265:THR:CG2	1:C:265:THR:O	2.65	0.43
1:D:134:LEU:HD23	1:D:157:TRP:CE3	2.54	0.43
1:C:151:GLN:O	1:C:155:GLN:HB2	2.18	0.43
1:B:29:LYS:HB3	1:B:29:LYS:HE2	1.94	0.43
1:A:31:VAL:HA	1:A:32:PRO:HD3	1.94	0.43
1:D:311:ILE:CD1	1:D:322:ILE:HD11	2.49	0.43
1:C:327:PHE:O	1:C:327:PHE:CG	2.69	0.43
1:D:48:LEU:CD2	1:D:49:SER:HB2	2.47	0.43
1:D:356:HIS:HD2	3:D:458:HOH:O	2.01	0.42
1:D:97:ALA:HB2	1:D:114:PHE:CZ	2.53	0.42
1:C:261:HIS:NE2	1:C:293:ASP:OD2	2.52	0.42
1:A:71:GLU:N	1:A:71:GLU:OE1	2.38	0.42
1:D:200:ARG:HH21	1:D:240:SER:HB3	1.83	0.42
1:C:354:ILE:HG22	1:C:356:HIS:CE1	2.54	0.42
1:A:249:LEU:HA	1:A:249:LEU:HD12	1.71	0.42
1:A:6:GLN:CA	1:A:6:GLN:HE21	2.30	0.42
1:C:267:THR:CG2	1:C:270:ASN:HB3	2.49	0.42
1:A:411:LYS:HB2	1:A:411:LYS:HE3	1.78	0.42
1:B:263:HIS:CD2	1:B:266:GLU:OE1	2.72	0.42
1:B:261:HIS:NE2	1:B:293:ASP:OD2	2.53	0.42
1:B:132:PRO:HD2	1:B:182:ASN:O	2.20	0.42
1:D:145:THR:HB	1:D:187:ASP:OD1	2.20	0.42
1:B:99:THR:O	1:B:99:THR:HG22	2.20	0.42
1:C:33:ILE:O	1:C:88:HIS:HB3	2.20	0.42
1:C:304:LEU:HD21	1:C:344:VAL:HA	2.01	0.42
1:D:137:HIS:CE1	1:D:139:LYS:HB2	2.54	0.42
1:B:249:LEU:CD2	1:B:279:HIS:CE1	3.02	0.42
1:C:36:HIS:HA	1:C:91:ASN:HB3	2.02	0.42
1:A:5:SER:O	1:A:9:ARG:HG2	2.20	0.42
1:C:231:ILE:HD13	1:C:231:ILE:N	2.35	0.42
1:D:42:ASP:C	1:D:43:VAL:HG23	2.40	0.42
1:D:14:TYR:CE2	1:D:386:ILE:HD12	2.53	0.41
1:A:14:TYR:CE2	1:A:386:ILE:HD11	2.55	0.41
1:D:404:LYS:O	1:D:408:ILE:HG23	2.21	0.41
1:D:80:ALA:O	1:D:84:ILE:HG13	2.20	0.41
1:C:79:LYS:HA	1:C:79:LYS:HD2	1.91	0.41
1:A:148:HIS:CD2	1:A:150:ASP:HB3	2.54	0.41
1:B:256:LEU:CD2	1:B:283:ALA:CB	2.96	0.41
1:A:413:VAL:O	1:A:416:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ASN:HD22	1:D:223:ALA:CB	2.28	0.41
1:D:271:LYS:O	1:D:275:MET:HG2	2.20	0.41
1:B:288:ARG:HA	1:B:289:PRO:HD2	1.99	0.41
1:A:292:TRP:NE1	1:A:294:SER:HB3	2.35	0.41
1:D:14:TYR:HE2	1:D:386:ILE:HD12	1.85	0.41
1:C:145:THR:HG22	1:C:146:LEU:N	2.15	0.41
1:B:87:LYS:HA	1:B:87:LYS:CE	2.47	0.41
1:D:334:ILE:N	1:D:334:ILE:CD1	2.84	0.41
1:C:280:ASP:O	1:C:319:ARG:HD2	2.20	0.41
1:A:143:GLY:O	1:A:187:ASP:HA	2.21	0.41
1:A:29:LYS:HA	1:A:390:TYR:OH	2.21	0.41
1:C:177:THR:HA	1:C:178:PRO:HD3	1.80	0.41
1:C:358:GLN:HE21	1:C:358:GLN:N	2.08	0.41
1:A:410:GLU:HA	1:A:414:LEU:CD2	2.51	0.41
1:C:234:GLU:H	1:C:234:GLU:HG2	1.53	0.41
1:A:400:GLU:O	1:A:401:GLU:C	2.58	0.40
1:A:168:GLY:O	1:A:171:PHE:HB2	2.22	0.40
1:D:354:ILE:HB	1:D:356:HIS:CE1	2.55	0.40
1:A:203:LEU:HD23	1:A:243:PHE:CE1	2.56	0.40
1:B:70:PRO:HD2	1:B:71:GLU:OE2	2.21	0.40
1:A:287:SER:HB3	1:A:325:ASP:O	2.21	0.40
1:A:4:LYS:HG3	1:A:6:GLN:CB	2.49	0.40
1:C:217:GLU:CD	1:C:217:GLU:N	2.72	0.40
1:A:354:ILE:HA	1:A:355:PRO:HD3	1.90	0.40
1:C:162:ILE:O	1:C:166:LYS:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	397/424 (94%)	377 (95%)	19 (5%)	1 (0%)	46 75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	398/424 (94%)	368 (92%)	30 (8%)	0	100	100
1	C	399/424 (94%)	379 (95%)	18 (4%)	2 (0%)	34	63
1	D	400/424 (94%)	373 (93%)	24 (6%)	3 (1%)	24	51
All	All	1594/1696 (94%)	1497 (94%)	91 (6%)	6 (0%)	39	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	300	PHE
1	C	145	THR
1	A	136	SER
1	D	136	SER
1	D	291	ARG
1	D	43	VAL

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	351/370 (95%)	308 (88%)	43 (12%)	6	14
1	B	351/370 (95%)	309 (88%)	42 (12%)	6	14
1	C	352/370 (95%)	313 (89%)	39 (11%)	8	17
1	D	353/370 (95%)	308 (87%)	45 (13%)	5	13
All	All	1407/1480 (95%)	1238 (88%)	169 (12%)	6	14

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	SER
1	A	6	GLN
1	A	11	LYS
1	A	16	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	27	ARG
1	A	31	VAL
1	A	43	VAL
1	A	48	LEU
1	A	77	LEU
1	A	87	LYS
1	A	93	HIS
1	A	99	THR
1	A	109	LEU
1	A	110	GLU
1	A	115	GLU
1	A	136	SER
1	A	145	THR
1	A	151	GLN
1	A	198	THR
1	A	205	GLU
1	A	209	GLN
1	A	228	LEU
1	A	276	LEU
1	A	281	LYS
1	A	284	LEU
1	A	313	ARG
1	A	315	ASP
1	A	321	LEU
1	A	324	LEU
1	A	338	THR
1	A	344	VAL
1	A	357	LYS
1	A	358	GLN
1	A	361	GLU
1	A	365	THR
1	A	379	LYS
1	A	383	LEU
1	A	400	GLU
1	A	403	LEU
1	A	413	VAL
1	A	414	LEU
1	A	416	GLN
1	B	4	LYS
1	B	5	SER
1	B	21	VAL
1	B	27	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	28	LEU
1	B	35	ILE
1	B	48	LEU
1	B	68	THR
1	B	75	MET
1	B	81	LEU
1	B	87	LYS
1	B	93	HIS
1	B	102	LYS
1	B	109	LEU
1	B	144	LEU
1	B	145	THR
1	B	177	THR
1	B	181	THR
1	B	187	ASP
1	B	214	GLU
1	B	217	GLU
1	B	249	LEU
1	B	250	LYS
1	B	254	LEU
1	B	256	LEU
1	B	267	THR
1	B	275	MET
1	B	281	LYS
1	B	294	SER
1	B	315	ASP
1	B	319	ARG
1	B	322	ILE
1	B	338	THR
1	B	346	LYS
1	B	348	LEU
1	B	357	LYS
1	B	358	GLN
1	B	365	THR
1	B	374	VAL
1	B	383	LEU
1	B	405	GLU
1	B	416	GLN
1	C	4	LYS
1	C	6	GLN
1	C	9	ARG
1	C	12	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	16	GLN
1	C	23	GLU
1	C	27	ARG
1	C	29	LYS
1	C	35	ILE
1	C	43	VAL
1	C	47	GLU
1	C	48	LEU
1	C	91	ASN
1	C	93	HIS
1	C	109	LEU
1	C	145	THR
1	C	173	LYS
1	C	179	CYS
1	C	187	ASP
1	C	192	THR
1	C	216	ASN
1	C	225	GLU
1	C	234	GLU
1	C	245	LEU
1	C	250	LYS
1	C	267	THR
1	C	276	LEU
1	C	282	LEU
1	C	286	VAL
1	C	291	ARG
1	C	321	LEU
1	C	338	THR
1	C	344	VAL
1	C	353	LEU
1	C	358	GLN
1	C	359	LEU
1	C	400	GLU
1	C	403	LEU
1	C	404	LYS
1	D	3	MET
1	D	5	SER
1	D	12	ILE
1	D	21	VAL
1	D	29	LYS
1	D	30	GLN
1	D	31	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	35	ILE
1	D	43	VAL
1	D	47	GLU
1	D	48	LEU
1	D	62	ASP
1	D	66	LYS
1	D	93	HIS
1	D	102	LYS
1	D	105	GLU
1	D	109	LEU
1	D	116	LYS
1	D	122	LYS
1	D	139	LYS
1	D	141	LYS
1	D	145	THR
1	D	146	LEU
1	D	176	GLU
1	D	177	THR
1	D	179	CYS
1	D	187	ASP
1	D	245	LEU
1	D	249	LEU
1	D	250	LYS
1	D	256	LEU
1	D	277	LEU
1	D	281	LYS
1	D	282	LEU
1	D	313	ARG
1	D	319	ARG
1	D	334	ILE
1	D	357	LYS
1	D	364	GLU
1	D	392	GLU
1	D	401	GLU
1	D	403	LEU
1	D	404	LYS
1	D	408	ILE
1	D	413	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	39	GLN
1	A	88	HIS
1	A	148	HIS
1	A	182	ASN
1	A	220	ASN
1	A	279	HIS
1	A	296	HIS
1	A	358	GLN
1	A	388	ASN
1	A	416	GLN
1	B	6	GLN
1	B	39	GLN
1	B	93	HIS
1	B	113	HIS
1	B	131	ASN
1	B	160	HIS
1	B	182	ASN
1	B	251	ASN
1	B	263	HIS
1	B	279	HIS
1	B	363	GLN
1	B	388	ASN
1	C	6	GLN
1	C	39	GLN
1	C	91	ASN
1	C	113	HIS
1	C	131	ASN
1	C	160	HIS
1	C	216	ASN
1	C	241	HIS
1	C	314	ASN
1	C	358	GLN
1	C	363	GLN
1	C	388	ASN
1	D	30	GLN
1	D	39	GLN
1	D	113	HIS
1	D	131	ASN
1	D	160	HIS
1	D	182	ASN
1	D	314	ASN
1	D	356	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](#)

Of 8 ligands modelled in this entry, 8 are 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/424 (94%)	-0.33	3 (0%) 89 90	16, 30, 45, 80	0
1	B	402/424 (94%)	-0.23	5 (1%) 81 81	16, 30, 50, 78	0
1	C	403/424 (95%)	-0.29	2 (0%) 91 93	19, 31, 45, 66	0
1	D	404/424 (95%)	-0.25	3 (0%) 89 90	19, 32, 54, 83	0
All	All	1610/1696 (94%)	-0.28	13 (0%) 87 88	16, 31, 50, 83	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	SER	5.7
1	B	4	LYS	3.7
1	C	4	LYS	3.3
1	C	49	SER	3.2
1	D	103	VAL	3.0
1	B	48	LEU	2.6
1	B	100	ASP	2.6
1	B	413	VAL	2.4
1	A	413	VAL	2.4
1	D	48	LEU	2.2
1	A	123	ARG	2.1
1	A	416	GLN	2.0
1	B	415	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	MN	B	420	1/1	0.93	0.25	3.98	63,63,63,63	0
2	MN	D	420	1/1	0.92	0.16	0.52	55,55,55,55	0
2	MN	A	420	1/1	0.83	0.16	-0.05	51,51,51,51	0
2	MN	C	419	1/1	0.75	0.15	-0.67	44,44,44,44	0
2	MN	B	419	1/1	0.84	0.15	-0.97	37,37,37,37	0
2	MN	D	419	1/1	0.97	0.11	-1.18	50,50,50,50	0
2	MN	A	419	1/1	0.95	0.12	-1.19	45,45,45,45	0
2	MN	C	420	1/1	0.82	0.12	-2.13	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.