Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 01:14 PM EST

PDB ID	:	3UXI
Title	:	Crystal structure of L-rhamnose isomerase W38A mutant from Bacillus halodurans
Authors	:	Doan, T.T.N.; Prabhu, P.; Kim, J.K.; Jeya, M.; Kang, L.W.; Lee, J.K.
Deposited on	:	2011-12-05
Resolution	:	2.73 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

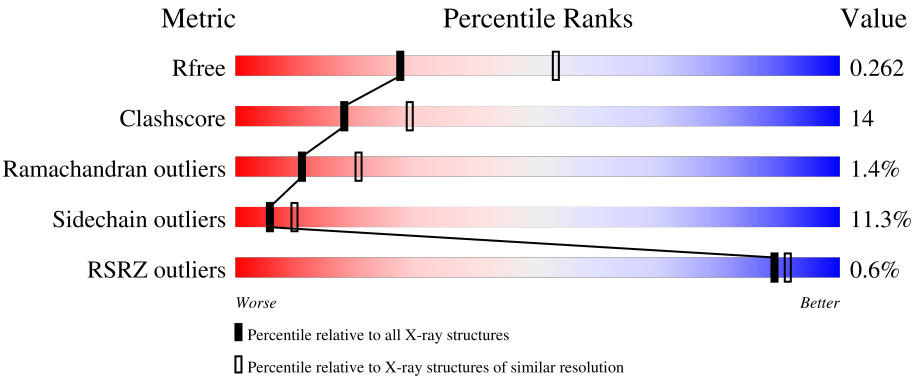
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	62% 27% 5% 5%
1	B	424	69% 21% • 5%
1	C	424	63% 26% 6% 5%
1	D	424	% 67% 24% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13410 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	402	Total	C	N	O	S	0	0	0
			3278	2098	564	607	9			
1	B	402	Total	C	N	O	S	0	0	0
			3278	2098	564	607	9			
1	C	404	Total	C	N	O	S	0	0	0
			3295	2109	567	609	10			
1	D	404	Total	C	N	O	S	0	0	0
			3295	2109	567	609	10			

There are 28 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
A	38	ALA	TRP	engineered mutation	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
B	38	ALA	TRP	engineered mutation	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
C	38	ALA	TRP	engineered mutation	UNP Q9KCL9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP Q9KCL9
D	-4	HIS	-	expression tag	UNP Q9KCL9
D	-3	HIS	-	expression tag	UNP Q9KCL9
D	-2	HIS	-	expression tag	UNP Q9KCL9
D	-1	HIS	-	expression tag	UNP Q9KCL9
D	0	HIS	-	expression tag	UNP Q9KCL9
D	38	ALA	TRP	engineered mutation	UNP Q9KCL9

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0

- Molecule 3 is water.

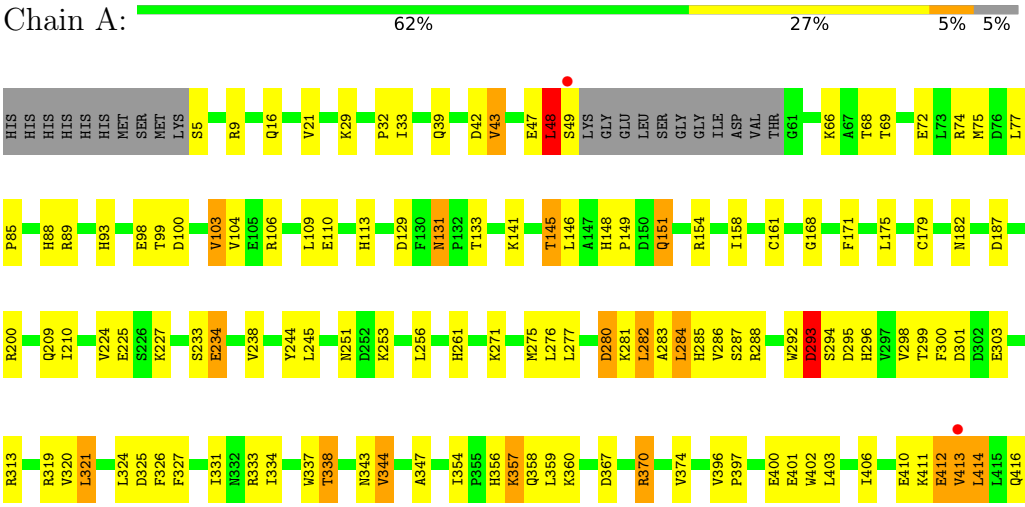
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	76	Total O 76 76	0	0
3	B	62	Total O 62 62	0	0
3	C	56	Total O 56 56	0	0
3	D	69	Total O 69 69	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

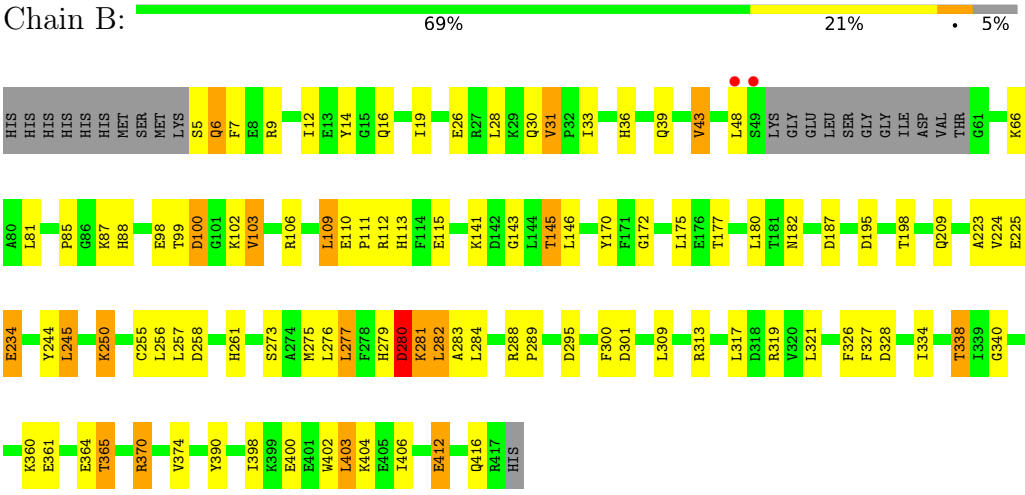
• Molecule 1: L-Rhamnose isomerase

Chain A:



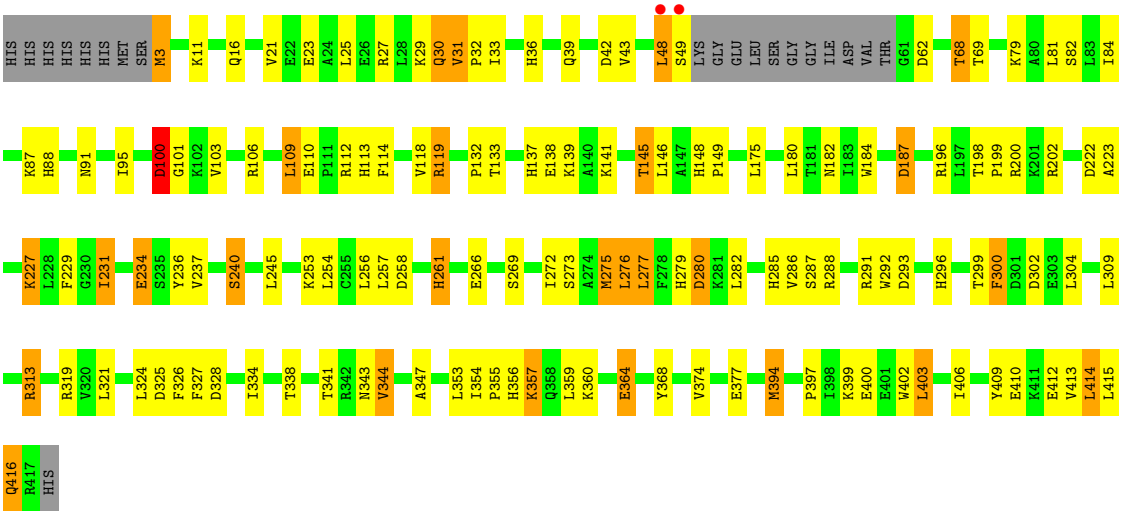
• Molecule 1: L-Rhamnose isomerase

Chain B:



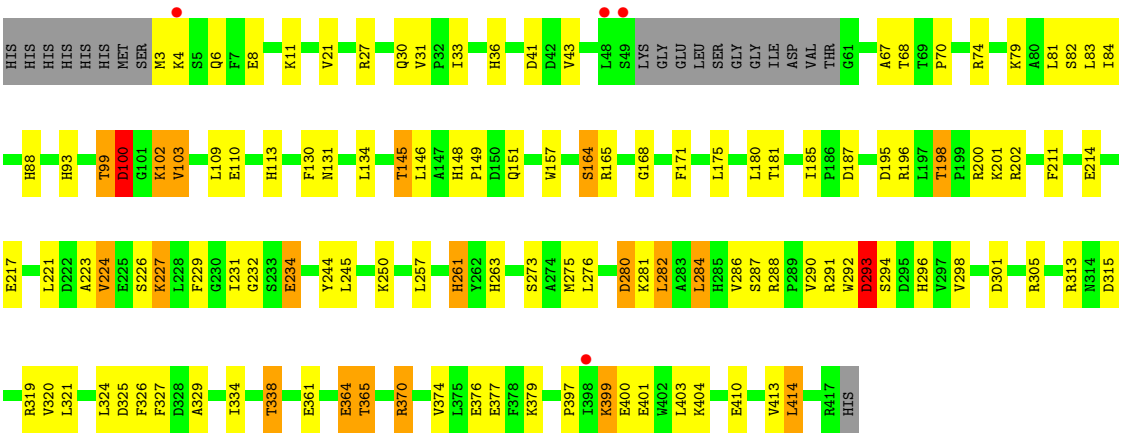
• Molecule 1: L-Rhamnose isomerase

Chain C:



- Molecule 1: L-Rhamnose isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.38Å 164.79Å 92.84Å 90.00° 117.02° 90.00°	Depositor
Resolution (Å)	45.87 – 2.73 45.87 – 2.73	Depositor EDS
% Data completeness (in resolution range)	82.5 (45.87-2.73) 82.5 (45.87-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.267 0.187 , 0.262	Depositor DCC
R_{free} test set	2480 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13410	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.82	1/3357 (0.0%)	0.83	4/4545 (0.1%)
1	B	0.72	1/3357 (0.0%)	0.82	2/4545 (0.0%)
1	C	0.77	0/3374	0.80	1/4566 (0.0%)
1	D	0.74	0/3374	0.82	5/4566 (0.1%)
All	All	0.76	2/13462 (0.0%)	0.82	12/18222 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	CYS	CB-SG	-6.10	1.71	1.82
1	A	234	GLU	CD-OE1	-5.05	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	293	ASP	CB-CG-OD2	6.74	124.36	118.30
1	B	284	LEU	CA-CB-CG	6.36	129.92	115.30
1	D	301	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	414	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	284	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	293	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	301	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	313	ARG	CB-CA-C	-5.46	99.49	110.40
1	A	99	THR	N-CA-C	-5.38	96.46	111.00
1	D	284	LEU	CA-CB-CG	5.24	127.35	115.30
1	C	277	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	414	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3278	0	3231	101	0
1	B	3278	0	3231	77	0
1	C	3295	0	3253	103	0
1	D	3295	0	3253	94	0
2	A	1	0	0	0	0
3	A	76	0	0	2	0
3	B	62	0	0	1	0
3	C	56	0	0	2	0
3	D	69	0	0	2	0
All	All	13410	0	12968	353	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 (353) 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:195:ASP:OD2	1:D:198:THR:HG23	1.50	1.12
1:A:410:GLU:HA	1:A:414:LEU:HB2	1.35	1.06
1:B:195:ASP:OD2	1:B:198:THR:HG22	1.55	1.05
1:C:245:LEU:HD22	1:D:245:LEU:HD22	1.43	1.00
1:D:286:VAL:HG23	1:D:298:VAL:HG21	1.46	0.95
1:C:110:GLU:H	1:C:113:HIS:HD2	1.13	0.95
1:C:245:LEU:HD22	1:D:245:LEU:CD2	1.96	0.94
1:A:286:VAL:HG23	1:A:298:VAL:HG21	1.51	0.92
1:D:287:SER:HB3	1:D:325:ASP:O	1.68	0.92
1:B:370:ARG:HG3	1:B:370:ARG:HH11	1.32	0.92
1:A:5:SER:HB2	3:A:458:HOH:O	1.70	0.91
1:D:148:HIS:ND1	1:D:149:PRO:HD2	1.88	0.89
1:A:110:GLU:H	1:A:113:HIS:HD2	1.19	0.88
1:C:145:THR:HG22	1:C:146:LEU:H	1.35	0.88
1:C:280:ASP:HA	1:C:319:ARG:NH1	1.89	0.87
1:D:195:ASP:OD2	1:D:198:THR:CG2	2.23	0.86
1:B:145:THR:CG2	1:B:146:LEU:H	1.89	0.85
1:A:261:HIS:CD2	1:A:293:ASP:OD2	2.28	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:HA	1:C:319:ARG:HH11	1.39	0.85
1:D:110:GLU:H	1:D:113:HIS:HD2	1.25	0.84
1:B:334:ILE:O	1:B:338:THR:HG23	1.77	0.84
1:D:370:ARG:HH11	1:D:370:ARG:HG3	1.44	0.82
1:A:85:PRO:O	1:A:88:HIS:HE1	1.60	0.82
1:A:334:ILE:O	1:A:338:THR:HG23	1.79	0.82
1:C:145:THR:CG2	1:C:146:LEU:H	1.92	0.82
1:D:334:ILE:O	1:D:338:THR:HG22	1.78	0.82
1:D:145:THR:HG22	1:D:146:LEU:N	1.96	0.81
1:B:145:THR:HG22	1:B:146:LEU:H	1.46	0.80
1:C:110:GLU:H	1:C:113:HIS:CD2	1.99	0.80
1:C:410:GLU:HA	1:C:414:LEU:HB2	1.61	0.80
1:B:110:GLU:H	1:B:113:HIS:HD2	1.27	0.79
1:D:134:LEU:HD23	1:D:145:THR:HG21	1.65	0.79
1:A:195:ASP:OD2	1:A:198:THR:CG2	2.31	0.79
1:B:145:THR:CG2	1:B:146:LEU:N	2.45	0.79
1:A:68:THR:HG22	1:A:69:THR:HG23	1.66	0.77
1:A:68:THR:HB	1:A:72:GLU:OE1	1.85	0.77
1:C:137:HIS:HE1	1:C:139:LYS:HG3	1.50	0.76
1:A:145:THR:HG22	1:A:146:LEU:H	1.49	0.76
1:D:257:LEU:HD11	1:D:275:MET:CE	2.14	0.76
1:B:195:ASP:CG	1:B:198:THR:HG22	2.05	0.76
1:D:370:ARG:HH11	1:D:370:ARG:CG	1.97	0.76
1:C:145:THR:CG2	1:C:146:LEU:N	2.50	0.74
1:D:280:ASP:O	1:D:319:ARG:HD2	1.87	0.74
1:D:334:ILE:O	1:D:338:THR:CG2	2.34	0.74
1:B:280:ASP:HA	1:B:319:ARG:NH1	2.02	0.74
1:A:110:GLU:H	1:A:113:HIS:CD2	2.05	0.73
1:A:145:THR:HG22	1:A:146:LEU:N	2.03	0.72
1:A:47:GLU:O	1:A:49:SER:N	2.23	0.72
1:D:33:ILE:H	1:D:88:HIS:HD2	1.35	0.72
1:C:137:HIS:CE1	1:C:139:LYS:HG3	2.25	0.71
1:A:145:THR:HB	1:A:187:ASP:OD1	1.91	0.71
1:C:198:THR:HB	1:C:199:PRO:HD3	1.72	0.71
1:C:198:THR:HB	1:C:199:PRO:CD	2.21	0.71
1:A:287:SER:HB3	1:A:325:ASP:O	1.92	0.69
1:A:295:ASP:HB3	1:A:327:PHE:H	1.56	0.69
1:D:130:PHE:CE2	1:D:164:SER:HB3	2.27	0.69
1:C:132:PRO:HD2	1:C:182:ASN:O	1.92	0.69
1:B:110:GLU:H	1:B:113:HIS:CD2	2.08	0.69
1:D:130:PHE:HE2	1:D:164:SER:HB3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:H	1:A:88:HIS:CD2	2.12	0.68
1:B:145:THR:HG23	1:B:146:LEU:N	2.09	0.68
1:B:102:LYS:O	1:B:103:VAL:HG12	1.94	0.67
1:C:79:LYS:O	1:C:82:SER:HB2	1.94	0.67
1:A:299:THR:HA	1:A:343:ASN:HD22	1.58	0.66
1:C:196:ARG:HG2	1:C:236:TYR:CE1	2.31	0.66
1:B:280:ASP:O	1:B:319:ARG:HD2	1.97	0.65
1:A:148:HIS:ND1	1:A:149:PRO:HD2	2.10	0.65
1:B:195:ASP:OD2	1:B:198:THR:CG2	2.37	0.65
1:B:370:ARG:HH11	1:B:370:ARG:CG	2.08	0.65
1:A:234:GLU:OE2	1:D:292:TRP:NE1	2.26	0.65
1:D:148:HIS:CE1	1:D:149:PRO:HD2	2.32	0.65
1:A:280:ASP:HA	1:A:319:ARG:NH1	2.13	0.64
1:A:33:ILE:H	1:A:88:HIS:HD2	1.42	0.64
1:A:261:HIS:NE2	1:A:293:ASP:OD2	2.31	0.64
1:D:130:PHE:O	1:D:181:THR:HA	1.96	0.64
1:D:145:THR:HB	1:D:187:ASP:OD1	1.97	0.64
1:B:280:ASP:HA	1:B:319:ARG:HH11	1.61	0.63
1:C:180:LEU:HD11	1:C:223:ALA:HB2	1.80	0.63
1:D:227:LYS:HA	1:D:261:HIS:HB3	1.80	0.63
1:A:85:PRO:O	1:A:88:HIS:CE1	2.49	0.63
1:D:324:LEU:HD13	1:D:326:PHE:CE2	2.33	0.62
1:B:279:HIS:O	1:B:280:ASP:CB	2.47	0.62
1:A:288:ARG:HB3	1:A:296:HIS:HB2	1.81	0.62
1:C:222:ASP:HB2	1:C:253:LYS:HD2	1.82	0.62
1:B:279:HIS:O	1:B:280:ASP:HB3	2.00	0.61
1:C:256:LEU:HD21	1:C:285:HIS:CG	2.36	0.61
1:C:231:ILE:O	1:C:231:ILE:HG13	2.00	0.61
1:C:356:HIS:O	1:C:360:LYS:HG3	2.01	0.61
1:D:324:LEU:HD13	1:D:326:PHE:HE2	1.65	0.61
1:A:292:TRP:O	1:A:294:SER:N	2.34	0.60
1:D:327:PHE:CZ	1:D:329:ALA:HB2	2.37	0.60
1:C:280:ASP:O	1:C:319:ARG:HD2	2.01	0.60
1:A:148:HIS:CG	1:A:149:PRO:HD2	2.37	0.59
1:C:39:GLN:HE22	1:C:328:ASP:H	1.50	0.59
1:A:195:ASP:OD2	1:A:198:THR:HG23	2.01	0.59
1:C:148:HIS:ND1	1:C:149:PRO:HD2	2.17	0.59
1:A:296:HIS:CE1	1:D:234:GLU:HG3	2.37	0.59
1:B:257:LEU:HD11	1:B:275:MET:CE	2.33	0.59
1:D:361:GLU:O	1:D:365:THR:HB	2.03	0.59
1:A:48:LEU:HD13	1:A:48:LEU:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:HG2	1:B:7:PHE:N	2.18	0.58
1:A:416:GLN:HG3	3:A:469:HOH:O	2.04	0.58
1:A:256:LEU:HA	1:A:283:ALA:O	2.04	0.57
1:D:134:LEU:HD22	1:D:185:ILE:HG22	1.85	0.57
1:D:286:VAL:HG23	1:D:298:VAL:CG2	2.27	0.57
1:A:145:THR:CG2	1:A:146:LEU:N	2.67	0.57
1:C:114:PHE:O	1:C:118:VAL:HG23	2.04	0.57
1:B:230:GLY:H	1:B:233:SER:HB3	1.69	0.57
1:A:367:ASP:OD2	1:A:370:ARG:HD3	2.04	0.57
1:D:165:ARG:NH1	1:D:211:PHE:HA	2.19	0.56
1:C:416:GLN:HE21	1:C:416:GLN:HA	1.69	0.56
1:C:287:SER:HB3	1:C:325:ASP:O	2.05	0.56
1:C:357:LYS:CD	1:C:357:LYS:H	2.16	0.56
1:D:280:ASP:OD1	1:D:281:LYS:N	2.38	0.56
1:B:400:GLU:O	1:B:403:LEU:HB2	2.05	0.56
1:A:299:THR:HA	1:A:343:ASN:ND2	2.20	0.56
1:D:83:LEU:HD22	1:D:397:PRO:HG2	1.87	0.56
1:A:412:GLU:HG2	1:A:413:VAL:HG22	1.87	0.56
1:D:27:ARG:HB2	3:D:456:HOH:O	2.06	0.56
1:C:68:THR:HG22	1:C:69:THR:HG23	1.87	0.56
1:A:106:ARG:HA	1:A:109:LEU:HD13	1.86	0.55
1:A:74:ARG:NH2	1:A:98:GLU:OE1	2.31	0.55
1:C:33:ILE:H	1:C:88:HIS:CD2	2.25	0.55
1:C:138:GLU:O	1:C:141:LYS:HG2	2.07	0.55
1:C:145:THR:HB	1:C:187:ASP:OD1	2.07	0.55
1:B:14:TYR:O	1:B:19:ILE:HB	2.07	0.55
1:B:106:ARG:HA	1:B:109:LEU:HD22	1.89	0.55
1:C:257:LEU:HD11	1:C:275:MET:CE	2.37	0.55
1:C:261:HIS:HE1	3:C:455:HOH:O	1.88	0.55
1:A:309:LEU:O	1:A:313:ARG:HB2	2.07	0.54
1:D:145:THR:CG2	1:D:146:LEU:N	2.68	0.54
1:A:85:PRO:HD3	1:A:396:VAL:HG21	1.90	0.54
1:C:145:THR:HG22	1:C:146:LEU:N	2.12	0.54
1:C:198:THR:N	1:C:199:PRO:HD2	2.21	0.54
1:D:261:HIS:CE1	1:D:293:ASP:OD2	2.61	0.54
1:D:280:ASP:HA	1:D:319:ARG:NH1	2.22	0.54
1:C:245:LEU:HD22	1:D:245:LEU:HD23	1.85	0.54
1:C:402:TRP:CZ3	1:C:403:LEU:HD13	2.43	0.54
1:D:145:THR:HG22	1:D:146:LEU:HG	1.90	0.54
1:A:245:LEU:HD22	1:B:245:LEU:HD22	1.90	0.54
1:C:334:ILE:HG22	1:C:406:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:HB3	1:A:238:VAL:HG21	1.91	0.53
1:A:197:LEU:HD11	1:B:277:LEU:CD1	2.39	0.53
1:A:104:VAL:CG2	1:A:109:LEU:HD12	2.39	0.53
1:D:226:SER:O	1:D:261:HIS:HD2	1.90	0.53
1:D:280:ASP:HA	1:D:319:ARG:HH11	1.74	0.53
1:A:227:LYS:HE2	1:A:261:HIS:CE1	2.43	0.53
1:D:180:LEU:HD12	1:D:221:LEU:O	2.09	0.53
1:B:334:ILE:HG22	1:B:406:ILE:HD12	1.90	0.53
1:D:102:LYS:O	1:D:103:VAL:HG12	2.09	0.53
1:D:148:HIS:ND1	1:D:149:PRO:CD	2.69	0.53
1:C:359:LEU:HD21	1:C:374:VAL:HG22	1.90	0.52
1:D:261:HIS:HE1	1:D:293:ASP:OD2	1.93	0.52
1:D:110:GLU:H	1:D:113:HIS:CD2	2.16	0.52
1:B:257:LEU:HD11	1:B:275:MET:HE3	1.91	0.52
1:D:8:GLU:OE1	1:D:11:LYS:HE2	2.10	0.52
1:A:168:GLY:O	1:A:171:PHE:HB2	2.10	0.52
1:C:261:HIS:CE1	1:C:293:ASP:OD2	2.62	0.52
1:C:400:GLU:O	1:C:403:LEU:HB2	2.10	0.52
1:B:234:GLU:OE1	1:C:292:TRP:NE1	2.42	0.52
1:B:361:GLU:O	1:B:365:THR:HB	2.09	0.52
1:C:148:HIS:CE1	1:C:149:PRO:HD2	2.45	0.52
1:A:303:GLU:O	1:A:307:ILE:HG13	2.10	0.52
1:D:196:ARG:HG3	1:D:196:ARG:HH11	1.75	0.52
1:A:197:LEU:HD11	1:B:277:LEU:HD13	1.92	0.51
1:A:77:LEU:O	1:A:81:LEU:HD22	2.09	0.51
1:C:229:PHE:HB2	1:C:234:GLU:HA	1.93	0.51
1:C:324:LEU:HD21	1:C:344:VAL:HG11	1.91	0.51
1:D:370:ARG:CG	1:D:370:ARG:NH1	2.64	0.51
1:B:98:GLU:C	1:B:99:THR:O	2.47	0.51
1:A:110:GLU:N	1:A:113:HIS:HD2	2.00	0.51
1:A:410:GLU:CA	1:A:414:LEU:HB2	2.26	0.51
1:B:172:GLY:HA2	1:B:177:THR:O	2.11	0.51
1:B:180:LEU:HD11	1:B:223:ALA:HB2	1.93	0.51
1:A:158:ILE:HG23	1:A:210:ILE:HG13	1.91	0.51
1:A:285:HIS:HB3	1:A:325:ASP:HB2	1.92	0.51
1:A:161:CYS:HB2	1:A:210:ILE:HG12	1.92	0.50
1:B:33:ILE:H	1:B:88:HIS:HD2	1.59	0.50
1:D:21:VAL:HG13	3:D:481:HOH:O	2.10	0.50
1:D:134:LEU:CD2	1:D:145:THR:HG21	2.39	0.50
1:D:232:GLY:N	1:D:234:GLU:OE2	2.35	0.50
1:B:256:LEU:HA	1:B:283:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:O	1:B:187:ASP:HA	2.11	0.50
1:A:234:GLU:CD	1:D:292:TRP:HE1	2.13	0.50
1:C:145:THR:HG23	1:C:146:LEU:N	2.26	0.50
1:A:357:LYS:CD	1:A:357:LYS:H	2.24	0.49
1:A:359:LEU:HD21	1:A:374:VAL:HG22	1.94	0.49
1:B:103:VAL:O	1:B:103:VAL:HG13	2.11	0.49
1:A:39:GLN:HB3	1:A:337:TRP:NE1	2.27	0.49
1:A:93:HIS:CE1	1:A:131:ASN:HB2	2.47	0.49
1:C:300:PHE:HE1	1:C:347:ALA:HA	1.77	0.49
1:B:230:GLY:N	1:B:233:SER:HB3	2.27	0.49
1:D:99:THR:O	1:D:100:ASP:O	2.30	0.49
1:A:400:GLU:HG3	1:C:377:GLU:HG3	1.94	0.49
1:B:85:PRO:O	1:B:88:HIS:HE1	1.95	0.49
1:A:42:ASP:OD2	1:A:333:ARG:NH2	2.45	0.49
1:A:370:ARG:O	1:A:374:VAL:HG13	2.13	0.49
1:D:410:GLU:HA	1:D:414:LEU:HB2	1.95	0.49
1:C:106:ARG:HA	1:C:109:LEU:HD22	1.95	0.48
1:A:66:LYS:HB3	1:A:333:ARG:CZ	2.43	0.48
1:B:224:VAL:HB	1:B:244:TYR:CD1	2.48	0.48
1:C:413:VAL:O	1:C:414:LEU:C	2.50	0.48
1:A:324:LEU:HD13	1:A:326:PHE:CE2	2.49	0.48
1:C:200:ARG:NH1	1:D:273:SER:OG	2.45	0.48
1:C:119:ARG:CB	1:C:119:ARG:HH11	2.27	0.48
1:B:31:VAL:HG11	1:B:317:LEU:HD22	1.96	0.48
1:C:95:ILE:CG2	1:C:133:THR:HG21	2.44	0.48
1:D:257:LEU:HD11	1:D:275:MET:HE2	1.94	0.48
1:B:43:VAL:HG12	1:B:43:VAL:O	2.14	0.47
1:B:111:PRO:HB3	1:B:170:TYR:CD2	2.49	0.47
1:A:321:LEU:N	1:A:321:LEU:CD1	2.78	0.47
1:B:39:GLN:HE22	1:B:328:ASP:H	1.62	0.47
1:B:402:TRP:CZ3	1:B:403:LEU:HD13	2.49	0.47
1:A:187:ASP:C	1:A:238:VAL:HG23	2.35	0.47
1:C:95:ILE:HG23	1:C:133:THR:HG21	1.96	0.47
1:D:290:VAL:O	1:D:291:ARG:HB2	2.15	0.47
1:D:292:TRP:O	1:D:294:SER:N	2.48	0.47
1:B:110:GLU:OE1	1:B:112:ARG:NH1	2.48	0.47
1:B:33:ILE:O	1:B:88:HIS:HB3	2.14	0.47
1:B:258:ASP:HB3	1:B:261:HIS:CG	2.50	0.47
1:B:412:GLU:O	1:B:416:GLN:HG3	2.15	0.47
1:D:102:LYS:O	1:D:103:VAL:CG1	2.63	0.47
1:A:413:VAL:O	1:A:414:LEU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:OD1	1:B:281:LYS:N	2.48	0.46
1:C:21:VAL:HG12	1:C:353:LEU:HD22	1.97	0.46
1:C:36:HIS:HA	1:C:91:ASN:HB3	1.97	0.46
1:D:145:THR:HG23	1:D:157:TRP:CD1	2.50	0.46
1:A:296:HIS:HE1	1:D:234:GLU:HG3	1.81	0.46
1:D:145:THR:HG23	1:D:157:TRP:CG	2.50	0.46
1:D:377:GLU:HA	1:D:377:GLU:OE1	2.15	0.46
1:A:48:LEU:N	1:A:48:LEU:CD1	2.78	0.46
1:B:111:PRO:HB3	1:B:170:TYR:CG	2.51	0.46
1:D:84:ILE:HG22	1:D:88:HIS:CE1	2.51	0.46
1:A:300:PHE:HE1	1:A:347:ALA:HA	1.81	0.46
1:C:266:GLU:HG3	1:D:263:HIS:CE1	2.51	0.46
1:D:168:GLY:O	1:D:171:PHE:HB2	2.16	0.46
1:B:334:ILE:HG22	1:B:406:ILE:CD1	2.46	0.46
1:D:195:ASP:CG	1:D:198:THR:HG23	2.29	0.46
1:A:227:LYS:HA	1:A:261:HIS:HB3	1.97	0.45
1:B:9:ARG:HD2	1:D:6:GLN:NE2	2.31	0.45
1:B:309:LEU:O	1:B:313:ARG:HG3	2.17	0.45
1:C:84:ILE:HG21	1:C:341:THR:HG21	1.97	0.45
1:B:33:ILE:N	1:B:88:HIS:HD2	2.13	0.45
1:A:301:ASP:HB2	1:C:302:ASP:OD2	2.16	0.45
1:A:417:ARG:H	1:A:417:ARG:HG3	1.51	0.45
1:A:148:HIS:ND1	1:A:149:PRO:CD	2.78	0.45
1:B:110:GLU:N	1:B:113:HIS:HD2	2.02	0.45
1:C:227:LYS:HA	1:C:261:HIS:HB3	1.98	0.45
1:A:9:ARG:NH1	1:C:3:MET:N	2.64	0.45
1:D:41:ASP:HB2	1:D:67:ALA:O	2.16	0.45
1:A:295:ASP:HB3	1:A:327:PHE:N	2.30	0.45
1:D:36:HIS:NE2	1:D:326:PHE:O	2.49	0.45
1:D:288:ARG:HB3	1:D:296:HIS:HB2	1.99	0.45
1:A:331:ILE:HG22	1:C:368:TYR:HB2	1.98	0.45
1:C:258:ASP:HB3	1:C:261:HIS:CG	2.52	0.45
1:C:309:LEU:O	1:C:313:ARG:HB3	2.17	0.45
1:D:134:LEU:HD23	1:D:145:THR:CG2	2.40	0.45
1:D:234:GLU:H	1:D:234:GLU:HG2	1.47	0.45
1:C:42:ASP:HA	1:C:327:PHE:CE2	2.52	0.45
1:C:257:LEU:HD11	1:C:275:MET:HE1	1.98	0.45
1:C:299:THR:HA	1:C:343:ASN:ND2	2.32	0.45
1:A:106:ARG:NH1	1:A:133:THR:O	2.50	0.45
1:D:148:HIS:CG	1:D:149:PRO:HD2	2.50	0.45
1:C:257:LEU:HD11	1:C:275:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:HIS:NE2	1:C:326:PHE:O	2.48	0.44
1:C:279:HIS:O	1:C:280:ASP:CG	2.56	0.44
1:D:224:VAL:HB	1:D:244:TYR:CD1	2.52	0.44
1:D:250:LYS:HA	1:D:250:LYS:HD2	1.77	0.44
1:A:271:LYS:HB3	1:A:275:MET:CE	2.47	0.44
1:D:110:GLU:N	1:D:113:HIS:HD2	2.05	0.44
1:A:129:ASP:HA	1:A:179:CYS:SG	2.58	0.44
1:C:413:VAL:O	1:C:415:LEU:N	2.50	0.44
1:D:282:LEU:O	1:D:320:VAL:HA	2.17	0.44
1:C:30:GLN:H	1:C:30:GLN:HG2	1.69	0.44
1:C:200:ARG:HH21	1:C:240:SER:HB3	1.82	0.44
1:A:397:PRO:HB2	1:A:402:TRP:HB3	2.00	0.44
1:B:229:PHE:CD1	1:C:291:ARG:HD2	2.53	0.44
1:D:70:PRO:HB2	1:D:74:ARG:NH2	2.33	0.44
1:A:357:LYS:H	1:A:357:LYS:HD3	1.82	0.44
1:B:33:ILE:H	1:B:88:HIS:CD2	2.36	0.44
1:C:288:ARG:HB3	1:C:296:HIS:HB2	2.00	0.43
1:A:271:LYS:HB3	1:A:275:MET:HE1	1.99	0.43
1:B:295:ASP:HB3	1:B:327:PHE:H	1.82	0.43
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.17	0.43
1:A:286:VAL:CG2	1:A:298:VAL:HG21	2.36	0.43
1:B:145:THR:HB	1:B:187:ASP:OD1	2.18	0.43
1:C:261:HIS:HE1	1:C:293:ASP:OD2	2.02	0.43
1:C:184:TRP:CZ2	1:C:227:LYS:HE3	2.54	0.43
1:C:364:GLU:CD	1:D:202:ARG:HH22	2.21	0.43
1:D:227:LYS:HD3	1:D:229:PHE:O	2.19	0.43
1:B:370:ARG:HG3	1:B:370:ARG:NH1	2.11	0.43
1:D:376:GLU:HA	1:D:379:LYS:HD2	2.01	0.43
1:C:256:LEU:HD11	1:C:285:HIS:NE2	2.34	0.43
1:D:305:ARG:HG3	1:D:305:ARG:NH1	2.34	0.42
1:A:151:GLN:HG2	1:A:154:ARG:NH2	2.35	0.42
1:B:275:MET:HG2	1:B:282:LEU:HD21	2.01	0.42
1:C:100:ASP:HB3	1:C:101:GLY:H	1.66	0.42
1:A:280:ASP:HA	1:A:319:ARG:HH11	1.81	0.42
1:D:399:LYS:HB3	1:D:400:GLU:H	1.63	0.42
1:C:110:GLU:HA	3:C:449:HOH:O	2.20	0.42
1:C:334:ILE:CG2	1:C:406:ILE:HD13	2.50	0.42
1:A:42:ASP:HA	1:A:327:PHE:CE2	2.55	0.42
1:D:82:SER:HB2	1:D:83:LEU:HG	2.02	0.42
1:D:226:SER:O	1:D:261:HIS:CD2	2.71	0.42
1:A:282:LEU:HD12	1:A:320:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:HIS:ND1	1:B:36:HIS:N	2.67	0.42
1:B:103:VAL:O	1:B:103:VAL:CG1	2.67	0.42
1:B:6:GLN:HG2	1:B:7:PHE:H	1.84	0.42
1:B:36:HIS:NE2	1:B:326:PHE:O	2.53	0.42
1:B:100:ASP:HB3	1:B:102:LYS:HG3	2.01	0.42
1:C:21:VAL:O	1:C:25:LEU:HG	2.20	0.42
1:D:305:ARG:HG3	1:D:305:ARG:HH11	1.85	0.42
1:A:196:ARG:O	1:A:200:ARG:HD2	2.20	0.41
1:B:68:THR:HG22	1:B:69:THR:HG23	2.00	0.41
1:C:33:ILE:H	1:C:88:HIS:HD2	1.65	0.41
1:C:222:ASP:O	1:C:254:LEU:HB2	2.20	0.41
1:C:334:ILE:HG22	1:C:406:ILE:HD11	2.02	0.41
1:A:310:GLU:OE2	1:A:313:ARG:NH1	2.53	0.41
1:A:356:HIS:O	1:A:360:LYS:HG3	2.21	0.41
1:B:250:LYS:HD3	1:B:250:LYS:HA	1.64	0.41
1:C:394:MET:HA	1:C:394:MET:CE	2.51	0.41
1:C:397:PRO:HG2	1:C:402:TRP:HA	2.03	0.41
1:A:104:VAL:HG22	1:A:109:LEU:HD12	2.01	0.41
1:B:182:ASN:HD21	1:B:225:GLU:HB2	1.84	0.41
1:C:11:LYS:HD3	1:C:21:VAL:CG2	2.51	0.41
1:A:357:LYS:HG2	1:A:358:GLN:OE1	2.20	0.41
1:C:304:LEU:HD21	1:C:344:VAL:HA	2.03	0.41
1:C:31:VAL:HA	1:C:32:PRO:HD3	1.68	0.41
1:C:377:GLU:OE1	1:C:377:GLU:HA	2.20	0.41
1:D:180:LEU:HD11	1:D:223:ALA:HB2	2.01	0.41
1:B:28:LEU:HD23	1:B:390:TYR:CZ	2.56	0.41
1:C:202:ARG:HH11	1:C:202:ARG:HD3	1.76	0.41
1:A:148:HIS:O	1:A:154:ARG:HD3	2.20	0.41
1:A:182:ASN:HD21	1:A:225:GLU:HB2	1.85	0.41
1:A:251:ASN:O	1:A:253:LYS:HG2	2.20	0.41
1:A:324:LEU:HD21	1:A:344:VAL:HG11	2.02	0.41
1:B:288:ARG:HA	1:B:289:PRO:HD2	1.94	0.41
1:C:272:ILE:HG22	1:C:276:LEU:HD22	2.02	0.41
1:C:273:SER:OG	1:D:200:ARG:NH1	2.54	0.41
1:C:409:TYR:CD2	1:C:414:LEU:HG	2.56	0.41
1:D:33:ILE:H	1:D:88:HIS:CD2	2.25	0.41
1:A:224:VAL:HB	1:A:244:TYR:CD1	2.56	0.41
1:A:234:GLU:HB3	1:D:290:VAL:HB	2.02	0.41
1:B:300:PHE:HE1	1:B:347:ALA:HA	1.86	0.41
1:B:340:GLY:O	1:B:344:VAL:HG12	2.21	0.41
1:C:33:ILE:O	1:C:88:HIS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ILE:CD1	1:D:292:TRP:CZ3	3.04	0.40
1:C:109:LEU:HD12	1:C:113:HIS:CD2	2.56	0.40
1:C:227:LYS:HG2	1:C:261:HIS:CG	2.56	0.40
1:A:32:PRO:HA	1:A:88:HIS:HD2	1.85	0.40
1:B:319:ARG:NH2	3:B:454:HOH:O	2.55	0.40
1:C:119:ARG:HH11	1:C:119:ARG:HB3	1.86	0.40
1:C:354:ILE:HG23	1:C:355:PRO:HD2	2.02	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	A	398/424 (94%)	359 (90%)	33 (8%)	6 (2%)	10 18
1	B	398/424 (94%)	367 (92%)	27 (7%)	4 (1%)	15 28
1	C	400/424 (94%)	370 (92%)	22 (6%)	8 (2%)	7 13
1	D	400/424 (94%)	365 (91%)	30 (8%)	5 (1%)	12 21
All	All	1596/1696 (94%)	1461 (92%)	112 (7%)	23 (1%)	11 20

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	B	100	ASP
1	B	280	ASP
1	C	412	GLU
1	D	100	ASP
1	A	103	VAL
1	C	100	ASP
1	C	112	ARG

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Mol	Chain	Res	Type
1	D	364	GLU
1	A	29	LYS
1	B	103	VAL
1	C	62	ASP
1	C	414	LEU
1	D	293	ASP
1	A	293	ASP
1	A	100	ASP
1	C	300	PHE
1	C	48	LEU
1	D	399	LYS
1	D	103	VAL
1	B	43	VAL
1	A	43	VAL
1	C	43	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	350/369 (95%)	314 (90%)	36 (10%)	7 13
1	B	350/369 (95%)	311 (89%)	39 (11%)	6 10
1	C	352/369 (95%)	310 (88%)	42 (12%)	5 8
1	D	352/369 (95%)	311 (88%)	41 (12%)	5 9
All	All	1404/1476 (95%)	1246 (89%)	158 (11%)	6 10

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	VAL
1	A	43	VAL
1	A	48	LEU
1	A	75	MET
1	A	79	LYS

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Mol	Chain	Res	Type
1	A	81	LEU
1	A	89	ARG
1	A	103	VAL
1	A	131	ASN
1	A	141	LYS
1	A	145	THR
1	A	151	GLN
1	A	175	LEU
1	A	198	THR
1	A	209	GLN
1	A	233	SER
1	A	276	LEU
1	A	277	LEU
1	A	280	ASP
1	A	281	LYS
1	A	282	LEU
1	A	284	LEU
1	A	310	GLU
1	A	321	LEU
1	A	338	THR
1	A	344	VAL
1	A	354	ILE
1	A	357	LYS
1	A	370	ARG
1	A	401	GLU
1	A	403	LEU
1	A	406	ILE
1	A	411	LYS
1	A	412	GLU
1	A	413	VAL
1	B	5	SER
1	B	6	GLN
1	B	12	ILE
1	B	16	GLN
1	B	30	GLN
1	B	31	VAL
1	B	48	LEU
1	B	66	LYS
1	B	79	LYS
1	B	81	LEU
1	B	87	LYS
1	B	109	LEU

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Mol	Chain	Res	Type
1	B	115	GLU
1	B	141	LYS
1	B	145	THR
1	B	175	LEU
1	B	209	GLN
1	B	234	GLU
1	B	245	LEU
1	B	250	LYS
1	B	273	SER
1	B	276	LEU
1	B	277	LEU
1	B	280	ASP
1	B	281	LYS
1	B	282	LEU
1	B	321	LEU
1	B	338	THR
1	B	344	VAL
1	B	357	LYS
1	B	360	LYS
1	B	364	GLU
1	B	365	THR
1	B	370	ARG
1	B	374	VAL
1	B	398	ILE
1	B	403	LEU
1	B	404	LYS
1	B	412	GLU
1	C	3	MET
1	C	16	GLN
1	C	23	GLU
1	C	27	ARG
1	C	29	LYS
1	C	30	GLN
1	C	31	VAL
1	C	48	LEU
1	C	49	SER
1	C	68	THR
1	C	81	LEU
1	C	87	LYS
1	C	100	ASP
1	C	103	VAL
1	C	109	LEU

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Mol	Chain	Res	Type
1	C	119	ARG
1	C	145	THR
1	C	175	LEU
1	C	187	ASP
1	C	227	LYS
1	C	231	ILE
1	C	234	GLU
1	C	237	VAL
1	C	240	SER
1	C	261	HIS
1	C	269	SER
1	C	275	MET
1	C	276	LEU
1	C	277	LEU
1	C	280	ASP
1	C	282	LEU
1	C	286	VAL
1	C	313	ARG
1	C	321	LEU
1	C	338	THR
1	C	344	VAL
1	C	357	LYS
1	C	364	GLU
1	C	394	MET
1	C	399	LYS
1	C	403	LEU
1	C	416	GLN
1	D	3	MET
1	D	4	LYS
1	D	30	GLN
1	D	31	VAL
1	D	43	VAL
1	D	68	THR
1	D	79	LYS
1	D	81	LEU
1	D	93	HIS
1	D	99	THR
1	D	100	ASP
1	D	102	LYS
1	D	109	LEU
1	D	131	ASN
1	D	145	THR

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Mol	Chain	Res	Type
1	D	151	GLN
1	D	164	SER
1	D	175	LEU
1	D	198	THR
1	D	201	LYS
1	D	214	GLU
1	D	217	GLU
1	D	224	VAL
1	D	227	LYS
1	D	234	GLU
1	D	261	HIS
1	D	276	LEU
1	D	280	ASP
1	D	282	LEU
1	D	284	LEU
1	D	315	ASP
1	D	321	LEU
1	D	338	THR
1	D	364	GLU
1	D	365	THR
1	D	370	ARG
1	D	374	VAL
1	D	401	GLU
1	D	403	LEU
1	D	404	LYS
1	D	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	39	GLN
1	A	88	HIS
1	A	113	HIS
1	A	182	ASN
1	A	388	ASN
1	A	416	GLN
1	B	39	GLN
1	B	88	HIS
1	B	113	HIS
1	B	182	ASN
1	B	314	ASN

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Mol	Chain	Res	Type
1	B	388	ASN
1	C	39	GLN
1	C	88	HIS
1	C	113	HIS
1	C	182	ASN
1	C	209	GLN
1	C	261	HIS
1	C	388	ASN
1	C	416	GLN
1	D	6	GLN
1	D	30	GLN
1	D	88	HIS
1	D	113	HIS
1	D	182	ASN
1	D	261	HIS
1	D	388	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	402/424 (94%)	-0.57	2 (0%)	91	93	16, 28, 47, 73	0
1	B	402/424 (94%)	-0.59	2 (0%)	91	93	18, 30, 42, 62	0
1	C	404/424 (95%)	-0.51	2 (0%)	91	93	16, 31, 49, 66	0
1	D	404/424 (95%)	-0.49	4 (0%)	82	86	17, 31, 54, 71	0
All	All	1612/1696 (95%)	-0.54	10 (0%)	89	91	16, 30, 49, 73	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	SER	5.5
1	C	49	SER	4.4
1	B	49	SER	3.4
1	D	48	LEU	2.7
1	C	48	LEU	2.6
1	A	413	VAL	2.5
1	D	4	LYS	2.3
1	B	48	LEU	2.3
1	D	398	ILE	2.2
1	A	49	SER	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	MN	A	419	1/1	0.83	0.14	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.