Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 12:14 PM EST

PDB ID	:	6M7Y
Title	:	Dehydratase, NisB, bound to a non-eliminable substrate analog
Authors	:	Cogan, D.P.; Nair, S.K.
Deposited on	:	2018-08-21
Resolution	:	2.79 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 (i) 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 (1)) were used in the production of this report:

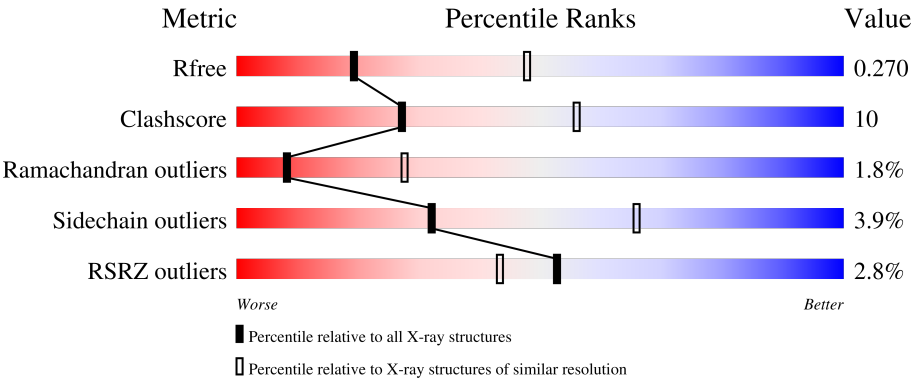
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	996	2% 72% 21%
1	B	996	4% 72% 21% 5%
2	C	34	6% 26% 9% 12% 53%
2	D	34	3% 29% 6% 12% 53%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16392 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 Nisin biosynthesis protein NisB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	952	Total	C	N	O	S	Se	0	1	0
			7947	5125	1298	1502	9	13			
1	B	948	Total	C	N	O	S	Se	0	7	0
			7944	5119	1299	1503	10	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P20103
A	-1	SER	-	expression tag	UNP P20103
A	0	HIS	-	expression tag	UNP P20103
A	1	MSE	-	expression tag	UNP P20103
A	169	CYS	VAL	engineered mutation	UNP P20103
B	-2	GLY	-	expression tag	UNP P20103
B	-1	SER	-	expression tag	UNP P20103
B	0	HIS	-	expression tag	UNP P20103
B	1	MSE	-	expression tag	UNP P20103
B	169	CYS	VAL	engineered mutation	UNP P20103

- Molecule 2 is a protein called Lantibiotic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	S	0	0	0
			127	81	21	24	1			
2	D	16	Total	C	N	O	S	0	0	0
			127	81	21	24	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	CYS	SER	engineered mutation	UNP Q7BB86
C	3	J9A	SER	engineered mutation	UNP Q7BB86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	ALA	CYS	engineered mutation	UNP Q7BB86
C	11	ALA	CYS	engineered mutation	UNP Q7BB86
D	-12	CYS	SER	engineered mutation	UNP Q7BB86
D	3	J9A	SER	engineered mutation	UNP Q7BB86
D	7	ALA	CYS	engineered mutation	UNP Q7BB86
D	11	ALA	CYS	engineered mutation	UNP Q7BB86

- Molecule 3 is water.

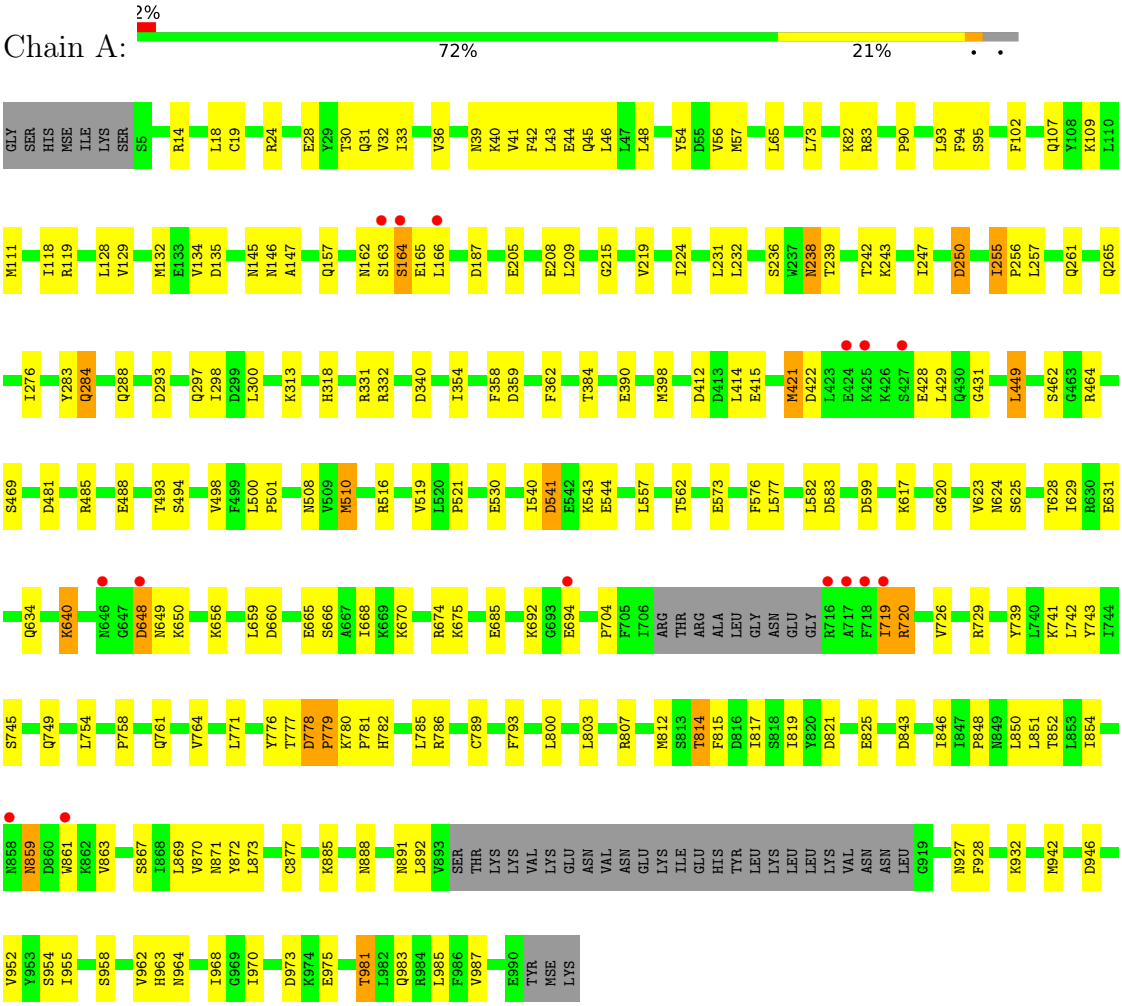
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	126	Total O 126 126	0	0
3	B	116	Total O 116 116	0	0
3	C	2	Total O 2 2	0	0
3	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

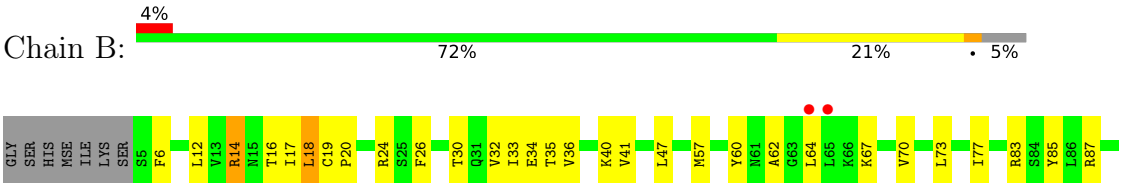
• Molecule 1: Nisin biosynthesis protein NisB

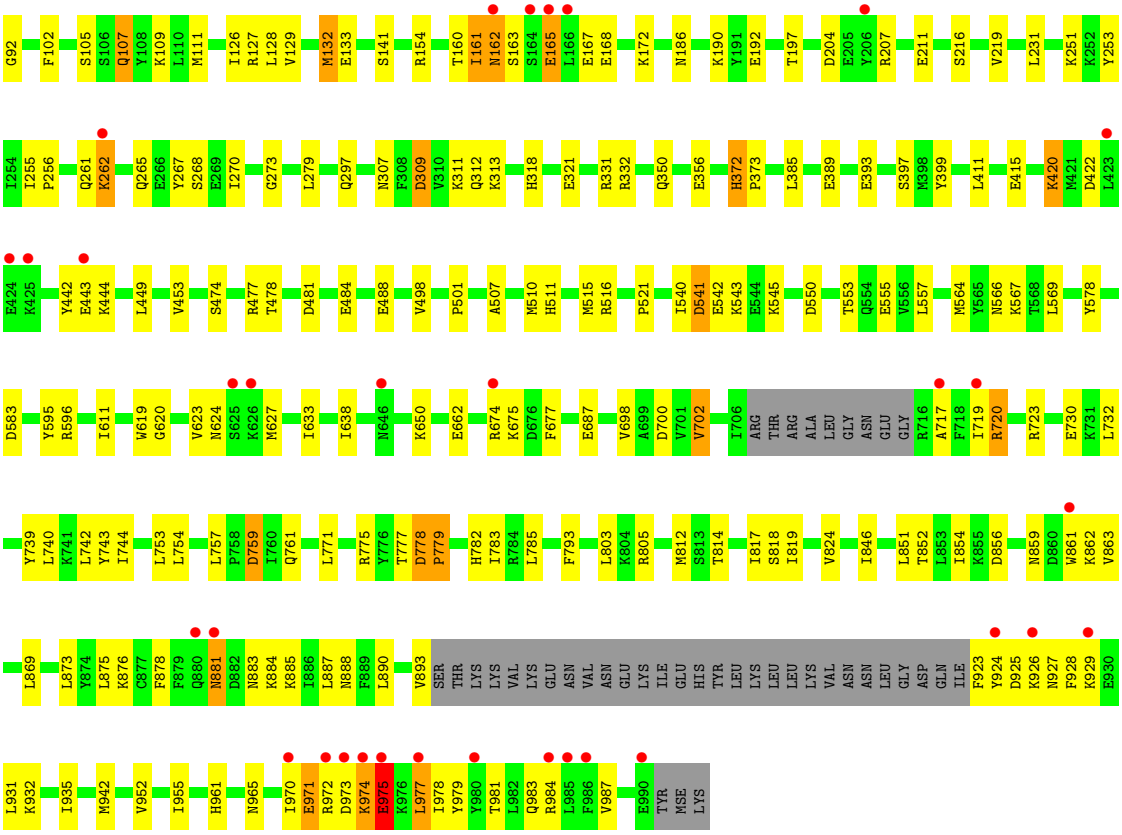
Chain A:



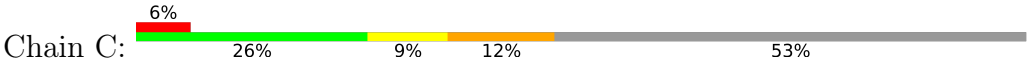
• Molecule 1: Nisin biosynthesis protein NisB

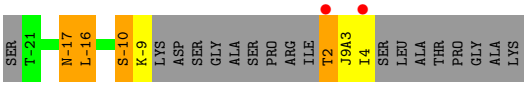
Chain B:



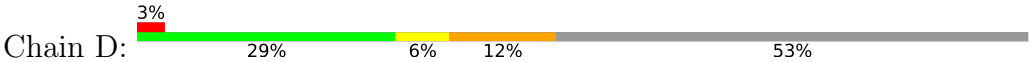


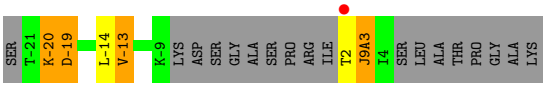
• Molecule 2: Lantibiotic





• Molecule 2: Lantibiotic





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.64Å 107.14Å 135.44Å 90.00° 109.57° 90.00°	Depositor
Resolution (Å)	29.39 – 2.79 29.39 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.39-2.79) 93.1 (29.39-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.185 , 0.270 0.188 , 0.270	Depositor DCC
R_{free} test set	3032 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16392	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: J9A

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	0.52	0/8095	0.66	0/10892
1	B	0.51	0/8092	0.70	7/10893 (0.1%)
2	C	0.59	0/110	0.68	0/144
2	D	0.49	0/110	0.59	0/144
All	All	0.51	0/16407	0.68	7/22073 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	975	GLU	N-CA-CB	19.37	145.46	110.60
1	B	372	HIS	C-N-CD	-10.41	97.69	120.60
1	B	974	LYS	N-CA-C	-10.00	83.99	111.00
1	B	975	GLU	N-CA-C	-8.76	87.36	111.00
1	B	132	MSE	CG-SE-CE	8.54	117.68	98.90
1	B	161	ILE	N-CA-C	-6.95	92.24	111.00
1	B	541	ASP	CB-CA-C	-5.42	99.57	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	372	HIS	Peptide
2	C	2	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7947	0	7907	146	0
1	B	7944	0	7866	179	0
2	C	127	0	113	4	0
2	D	127	0	114	6	0
3	A	126	0	0	4	0
3	B	116	0	0	3	0
3	C	2	0	0	0	0
3	D	3	0	0	1	0
All	All	16392	0	16000	324	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 10.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LEU:HD23	1:B:978:ILE:HG13	1.42	1.00
1:A:628:THR:HG22	1:A:631:GLU:OE1	1.68	0.93
1:B:977:LEU:CD2	1:B:978:ILE:HG13	1.98	0.93
1:B:261[B]:GLN:HG3	1:B:262:LYS:HD3	1.51	0.92
1:A:232:LEU:HD13	1:A:510:MSE:HE1	1.50	0.91
1:A:970:ILE:HG13	2:D:2:THR:HA	1.58	0.85
1:B:165:GLU:OE2	3:B:1001:HOH:O	1.95	0.84
1:B:541:ASP:HB3	1:B:543:LYS:H	1.43	0.84
1:A:628:THR:HG22	1:A:631:GLU:CD	2.01	0.81
1:A:208:GLU:HG3	1:A:209:LEU:H	1.45	0.80
1:B:719:ILE:HG13	1:B:720:ARG:H	1.47	0.79
1:A:628:THR:CG2	1:A:631:GLU:OE1	2.31	0.78
1:B:961:HIS:ND1	1:B:975:GLU:OE2	2.20	0.75
1:A:942:MSE:HE3	1:A:955:ILE:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:ASP:O	1:B:859:ASN:ND2	2.21	0.73
1:B:925:ASP:OD1	1:B:926:LYS:N	2.21	0.73
1:B:541:ASP:HB2	1:B:545:LYS:H	1.54	0.72
1:B:754:LEU:HD22	1:B:852:THR:HG23	1.71	0.72
1:B:255:ILE:HG13	1:B:256:PRO:HD3	1.70	0.72
1:A:859:ASN:OD1	1:A:861:TRP:HE3	1.73	0.72
1:B:553:THR:OG1	1:B:555:GLU:HG3	1.89	0.72
1:B:942:MSE:HE3	1:B:955:ILE:HD12	1.71	0.71
1:A:891:ASN:OD1	1:A:892:LEU:HG	1.90	0.71
1:A:803:LEU:HD22	1:A:812:MSE:HE1	1.71	0.71
2:D:-20:LYS:HE2	2:D:-20:LYS:HA	1.72	0.71
1:B:873:LEU:HD21	1:B:928:PHE:HD2	1.56	0.70
1:A:481:ASP:O	1:A:485:ARG:HG2	1.92	0.69
1:B:18:LEU:HD21	1:B:41:VAL:HG21	1.74	0.69
1:A:318:HIS:NE2	1:A:415:GLU:OE1	2.24	0.69
1:A:648:ASP:OD1	1:A:649:ASN:ND2	2.27	0.68
1:B:87[B]:ARG:HG3	1:B:87[B]:ARG:HH11	1.59	0.67
1:B:356:GLU:OE2	1:B:723:ARG:NH1	2.29	0.66
1:B:977:LEU:HD23	1:B:978:ILE:H	1.61	0.66
1:B:777:THR:HG23	1:B:970:ILE:HD13	1.78	0.66
1:B:942:MSE:HE2	1:B:952:VAL:HG22	1.78	0.65
1:A:814:THR:HG22	1:B:819:ILE:HD12	1.78	0.65
1:B:41:VAL:HG12	1:B:273:GLY:HA3	1.78	0.65
1:B:803:LEU:HD22	1:B:812:MSE:HE1	1.79	0.65
1:B:884:LYS:O	1:B:888:ASN:ND2	2.30	0.64
1:A:543:LYS:O	1:A:543:LYS:HG3	1.97	0.64
1:B:331:ARG:HB2	1:B:385:LEU:HD23	1.78	0.64
1:B:977:LEU:O	1:B:981:THR:HG23	1.98	0.64
1:B:977:LEU:CD2	1:B:978:ILE:CG1	2.73	0.64
1:B:742:LEU:HB3	1:B:812:MSE:HE2	1.80	0.63
1:A:629:ILE:HD12	1:A:629:ILE:H	1.64	0.62
1:B:566:ASN:HB3	1:B:569:LEU:HD12	1.81	0.62
1:B:942:MSE:HE1	1:B:952:VAL:HA	1.80	0.62
1:B:977:LEU:HD21	1:B:978:ILE:CG1	2.30	0.62
1:A:942:MSE:HE1	1:A:952:VAL:HA	1.81	0.61
1:A:28:GLU:O	1:A:32:VAL:HG23	2.00	0.61
1:B:102:PHE:CD1	1:B:313:LYS:HB2	2.35	0.61
1:B:624:ASN:OD1	1:B:627:MSE:N	2.34	0.61
1:B:873:LEU:CD2	1:B:928:PHE:CD2	2.84	0.61
1:A:848:PRO:O	1:A:852:THR:HG23	2.01	0.60
1:A:24:ARG:NH2	1:A:31:GLN:HE21	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:HD11	1:A:785:LEU:HD12	1.83	0.60
1:A:82:LYS:NZ	1:A:660:ASP:OD1	2.33	0.60
1:B:971:GLU:HG2	1:B:974:LYS:HB2	1.83	0.60
1:A:165:GLU:CD	1:A:166:LEU:H	2.04	0.60
1:A:628:THR:OG1	1:A:629:ILE:N	2.35	0.60
1:B:893:VAL:HG11	1:B:979:TYR:CD2	2.37	0.60
1:B:961:HIS:NE2	2:C:2:THR:HA	2.16	0.60
1:A:541:ASP:HB3	1:A:543:LYS:H	1.67	0.59
1:B:20:PRO:HB2	1:B:687:GLU:OE2	2.02	0.59
1:A:128:LEU:HD11	1:A:132:MSE:HE3	1.84	0.59
1:A:620:GLY:O	1:A:623:VAL:HG22	2.02	0.59
1:B:109:LYS:O	1:B:111:MSE:HE2	2.03	0.59
1:A:540:ILE:CG2	1:A:544:GLU:HA	2.32	0.59
1:B:507:ALA:O	1:B:510:MSE:HG2	2.02	0.58
1:A:666:SER:O	1:A:670:LYS:HG3	2.02	0.58
1:B:109:LYS:HE2	1:B:111:MSE:SE	2.53	0.58
1:B:983:GLN:O	1:B:987:VAL:HG23	2.03	0.58
1:A:494:SER:OG	1:A:516:ARG:HG3	2.02	0.58
1:B:207:ARG:O	1:B:211:GLU:HG3	2.03	0.58
1:A:39:ASN:O	1:A:43:LEU:HD12	2.04	0.58
1:B:47:LEU:HD23	1:B:279:LEU:HD23	1.85	0.58
1:A:629:ILE:HG12	1:A:668:ILE:HG21	1.85	0.58
1:A:867:SER:O	1:A:871:ASN:ND2	2.29	0.57
1:B:484:GLU:O	1:B:488:GLU:HG3	2.03	0.57
1:B:550:ASP:HB2	1:B:557:LEU:HD11	1.86	0.57
1:A:208:GLU:HG3	1:A:209:LEU:N	2.16	0.57
1:B:873:LEU:CD2	1:B:928:PHE:HD2	2.17	0.57
1:A:255:ILE:HB	1:A:256:PRO:HD3	1.87	0.57
1:A:24:ARG:HH21	1:A:31:GLN:HE21	1.51	0.56
1:A:239:THR:O	1:A:243:LYS:HG3	2.04	0.56
1:B:442:TYR:O	1:B:443:GLU:HG2	2.06	0.56
1:B:161:ILE:O	1:B:163:SER:N	2.38	0.56
2:C:4:ILE:HG23	2:C:4:ILE:O	2.05	0.56
1:B:761:GLN:HG3	1:B:771:LEU:HD21	1.88	0.55
1:B:859:ASN:OD1	1:B:861:TRP:N	2.39	0.55
1:A:18:LEU:HD21	1:A:41:VAL:HG11	1.87	0.55
1:B:854:ILE:HG21	1:B:863:VAL:HG13	1.87	0.55
1:B:876:LYS:HE3	1:B:881:ASN:HB3	1.88	0.55
1:B:981:THR:O	1:B:984:ARG:HG2	2.06	0.55
1:A:485:ARG:HH12	1:A:488:GLU:CD	2.09	0.55
1:B:129:VAL:O	1:B:133:GLU:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ARG:NH2	2:D:-13:VAL:HG13	2.22	0.55
1:B:885:LYS:HA	1:B:888:ASN:HD22	1.71	0.55
1:B:12:LEU:HB2	1:B:702:VAL:HG13	1.89	0.55
1:B:261[B]:GLN:HE21	1:B:261[B]:GLN:C	2.10	0.55
1:A:942:MSE:HE2	1:A:952:VAL:HG22	1.90	0.54
1:B:854:ILE:HD13	1:B:863:VAL:HG12	1.89	0.54
1:A:742:LEU:HB3	1:A:812:MSE:HE2	1.89	0.54
1:A:33:ILE:HG23	1:A:57:MSE:HE2	1.90	0.54
1:A:109:LYS:HE2	1:A:111:MSE:SE	2.58	0.53
1:B:443:GLU:HG3	1:B:444:LYS:CD	2.38	0.53
1:B:923:PHE:CE1	1:B:932:LYS:HD3	2.43	0.53
1:B:923:PHE:HE1	1:B:932:LYS:HD3	1.72	0.53
1:B:399:TYR:HB2	1:B:595:TYR:CE1	2.44	0.52
1:B:33:ILE:HG23	1:B:57:MSE:HE2	1.91	0.52
1:B:40:LYS:HG2	1:B:273:GLY:O	2.08	0.52
1:B:318:HIS:NE2	1:B:415:GLU:OE2	2.38	0.52
1:A:93:LEU:HA	1:A:300:LEU:HD11	1.91	0.52
1:B:41:VAL:HG12	1:B:273:GLY:CA	2.39	0.52
1:B:128:LEU:HD11	1:B:132:MSE:HE3	1.92	0.52
1:A:859:ASN:OD1	1:A:861:TRP:CE3	2.59	0.52
1:B:261[B]:GLN:O	1:B:261[B]:GLN:NE2	2.25	0.52
1:B:265:GLN:O	1:B:268:SER:HB3	2.10	0.52
1:B:510:MSE:HG3	1:B:511:HIS:N	2.23	0.52
1:A:854:ILE:HD13	1:A:863:VAL:HG23	1.92	0.51
1:B:18:LEU:HD21	1:B:41:VAL:CG2	2.40	0.51
1:A:500:LEU:HD12	1:A:501:PRO:HD2	1.92	0.51
1:A:983:GLN:O	1:A:987:VAL:HG23	2.10	0.51
1:A:215:GLY:O	1:A:219:VAL:HG23	2.09	0.51
1:A:354:ILE:HD12	1:A:577:LEU:HD21	1.92	0.51
1:B:172:LYS:HD3	3:D:101:HOH:O	2.11	0.51
1:B:923:PHE:O	1:B:923:PHE:CD1	2.63	0.51
1:B:675:LYS:HE2	1:B:675:LYS:HA	1.92	0.51
1:B:255:ILE:CG1	1:B:256:PRO:HD3	2.38	0.51
1:A:48:LEU:HA	1:A:283:TYR:OH	2.11	0.50
1:A:284:GLN:O	1:A:288:GLN:HG3	2.10	0.50
1:A:729:ARG:NH2	1:A:825:GLU:OE2	2.43	0.50
1:B:350:GLN:OE1	1:B:723:ARG:HD2	2.11	0.50
1:B:873:LEU:HD21	1:B:928:PHE:CD2	2.40	0.50
1:B:977:LEU:HD23	1:B:978:ILE:N	2.26	0.50
1:B:740:LEU:HD23	1:B:817:ILE:HG12	1.94	0.49
1:B:262:LYS:HA	1:B:265:GLN:HB3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:TYR:HA	1:B:270:ILE:HD12	1.94	0.49
1:B:854:ILE:HD13	1:B:863:VAL:HA	1.94	0.49
1:A:102:PHE:CD1	1:A:313:LYS:HB2	2.47	0.49
1:B:411:LEU:HD12	1:B:611:ILE:HG13	1.94	0.49
1:A:398:MSE:SE	1:A:414:LEU:HD11	2.63	0.49
1:A:332:ARG:NH2	1:A:340:ASP:OD2	2.40	0.49
1:A:485:ARG:NH1	1:A:488:GLU:OE2	2.40	0.49
1:A:778:ASP:N	1:A:779:PRO:O	2.45	0.49
1:A:877:CYS:SG	1:A:932:LYS:HG3	2.53	0.49
1:A:90:PRO:HA	1:A:95:SER:OG	2.13	0.49
1:A:970:ILE:CG1	2:D:2:THR:HA	2.38	0.48
1:B:754:LEU:HD21	1:B:851:LEU:HB2	1.95	0.48
1:A:764:VAL:HG21	1:A:771:LEU:HD23	1.95	0.48
1:A:778:ASP:HA	1:A:779:PRO:O	2.12	0.48
1:B:501:PRO:HG2	1:B:507:ALA:HA	1.95	0.48
1:A:779:PRO:HA	3:A:1036:HOH:O	2.13	0.48
1:B:62:ALA:O	1:B:64:LEU:HG	2.13	0.48
1:A:165:GLU:CD	1:A:166:LEU:N	2.67	0.48
1:B:477:ARG:HA	1:B:515:MSE:HE2	1.96	0.48
1:B:931:LEU:O	1:B:935:ILE:HG13	2.14	0.48
1:B:754:LEU:HD21	1:B:851:LEU:CB	2.44	0.48
1:B:778:ASP:HA	1:B:779:PRO:HA	1.47	0.48
1:B:805[A]:ARG:NH1	3:B:1007:HOH:O	2.41	0.48
1:B:443:GLU:HG3	1:B:444:LYS:HD2	1.95	0.47
1:A:250:ASP:OD1	1:A:250:ASP:N	2.48	0.47
1:B:128:LEU:CG	1:B:132:MSE:HE3	2.44	0.47
1:B:650:LYS:NZ	3:B:1006:HOH:O	2.38	0.47
1:A:390:GLU:HG3	3:A:1043:HOH:O	2.14	0.47
1:B:67:LYS:O	1:B:70:VAL:HG12	2.14	0.47
1:A:145:ASN:HA	1:A:224:ILE:HD12	1.97	0.47
1:A:165:GLU:OE1	1:A:166:LEU:N	2.48	0.47
1:A:494:SER:CB	1:A:516:ARG:HG3	2.45	0.47
1:A:36:VAL:HG13	1:A:42:PHE:CD1	2.49	0.47
1:A:284:GLN:HE21	1:A:288:GLN:NE2	2.13	0.47
1:A:631:GLU:HA	1:A:634:GLN:HB2	1.95	0.47
1:A:777:THR:HG23	1:A:970:ILE:HD13	1.97	0.47
1:B:619:TRP:CE3	1:B:677:PHE:HB3	2.50	0.47
1:B:753:LEU:HD22	1:B:757:LEU:HD22	1.96	0.47
1:B:775:ARG:HD2	1:B:965:ASN:O	2.13	0.47
1:B:542:GLU:HG2	1:B:543:LYS:N	2.28	0.47
1:A:870:VAL:HG11	1:A:963:HIS:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:O	1:A:276:ILE:HD11	2.15	0.47
1:B:442:TYR:C	1:B:443:GLU:HG2	2.35	0.47
1:A:498:VAL:O	1:A:521:PRO:HA	2.14	0.46
1:A:819:ILE:HD12	1:B:814:THR:HG22	1.97	0.46
1:B:633:ILE:HB	1:B:638:ILE:HG13	1.98	0.46
1:A:729:ARG:HD3	1:A:821:ASP:OD1	2.16	0.46
1:B:128:LEU:HG	1:B:132:MSE:HE3	1.96	0.46
1:A:885:LYS:O	1:A:888:ASN:HB2	2.15	0.46
1:B:128:LEU:CD1	1:B:132:MSE:HE3	2.46	0.46
1:A:162:ASN:O	1:A:164:SER:N	2.49	0.46
1:B:389:GLU:O	1:B:393:GLU:HG3	2.16	0.46
1:B:541:ASP:HB3	1:B:543:LYS:N	2.20	0.46
1:A:719:ILE:HG13	1:A:720:ARG:HD2	1.98	0.46
1:B:255:ILE:HG13	1:B:256:PRO:CD	2.44	0.46
1:B:674:ARG:HG3	1:B:674:ARG:O	2.15	0.46
1:B:743:TYR:CD2	1:B:782:HIS:HB3	2.51	0.46
1:A:800:LEU:HD11	1:B:732:LEU:HD13	1.97	0.45
1:A:743:TYR:CD1	1:A:782:HIS:HB3	2.52	0.45
1:B:160:THR:HG23	1:B:162:ASN:HB2	1.97	0.45
1:A:118:ILE:HG12	1:A:298:ILE:HG12	1.97	0.45
1:A:629:ILE:HD13	1:A:665:GLU:OE2	2.16	0.45
1:B:977:LEU:HG	1:B:978:ILE:N	2.31	0.45
1:B:846:ILE:HG22	1:B:927:ASN:HB3	1.98	0.45
1:A:331:ARG:NH2	1:A:421:MSE:HE2	2.31	0.45
1:A:359:ASP:OD2	1:A:362:PHE:N	2.49	0.45
1:A:807:ARG:NH1	1:B:730:GLU:OE2	2.44	0.45
1:A:873:LEU:HB3	1:A:928:PHE:CZ	2.52	0.45
1:B:474:SER:O	1:B:478:THR:HG23	2.17	0.45
2:D:-19:ASP:OD1	2:D:-19:ASP:N	2.49	0.45
1:A:846:ILE:HG22	1:A:927:ASN:HB3	1.97	0.45
1:B:633:ILE:O	1:B:638:ILE:HG12	2.17	0.45
1:A:624:ASN:OD1	1:A:625:SER:N	2.50	0.45
1:B:477:ARG:HG3	1:B:515:MSE:HE1	1.98	0.45
1:A:297:GLN:OE1	1:A:508:ASN:HB3	2.16	0.45
1:B:161:ILE:HB	1:B:162:ASN:H	1.60	0.45
1:B:17:ILE:HD13	1:B:17:ILE:HA	1.79	0.44
1:B:18:LEU:HD13	1:B:85:TYR:CZ	2.52	0.44
1:B:854:ILE:HG23	1:B:862:LYS:HA	1.99	0.44
1:B:309:ASP:HB2	1:B:312[B]:GLN:HG2	1.98	0.44
1:A:429:LEU:HD11	1:A:431:GLY:O	2.17	0.44
1:A:668:ILE:HD12	1:A:668:ILE:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:HD3	1:B:700:ASP:OD1	2.18	0.44
1:B:141:SER:HB3	1:B:190:LYS:HA	2.00	0.44
1:A:786:ARG:NH2	2:D:3:J9A:O01	2.39	0.44
1:B:216:SER:HA	1:B:219:VAL:HG12	1.99	0.44
1:B:620:GLY:O	1:B:623:VAL:HG12	2.18	0.44
1:A:242:THR:HG21	3:A:1102:HOH:O	2.18	0.44
1:A:261:GLN:O	1:A:265:GLN:HG3	2.18	0.44
1:B:873:LEU:CD2	1:B:928:PHE:CE2	3.00	0.44
1:A:332:ARG:HG2	1:A:384:THR:HA	2.00	0.44
1:A:741:LYS:O	1:A:815:PHE:HA	2.18	0.44
1:A:869:LEU:O	1:A:872:TYR:HB3	2.17	0.44
1:A:428:GLU:HB3	1:A:583:ASP:OD1	2.18	0.43
1:B:57:MSE:HE3	1:B:77:ILE:HG13	1.99	0.43
1:B:261[B]:GLN:CG	1:B:262:LYS:HD3	2.36	0.43
1:A:540:ILE:HG23	1:A:544:GLU:HA	1.99	0.43
1:A:147:ALA:O	1:A:157:GLN:HA	2.17	0.43
1:A:358:PHE:HZ	1:A:576:PHE:CG	2.36	0.43
1:A:659:LEU:HD23	1:A:659:LEU:HA	1.75	0.43
1:A:817:ILE:HB	1:B:817:ILE:HB	2.00	0.43
1:B:253:TYR:O	1:B:256:PRO:HD2	2.19	0.43
1:A:758:PRO:HA	1:A:761:GLN:HE21	1.82	0.43
1:A:778:ASP:CA	1:A:779:PRO:O	2.66	0.43
1:A:793:PHE:HB2	1:B:793:PHE:CZ	2.53	0.43
1:B:977:LEU:CG	1:B:978:ILE:N	2.81	0.43
1:B:32:VAL:O	1:B:36:VAL:HG22	2.19	0.43
1:B:420:LYS:HD2	1:B:420:LYS:C	2.38	0.43
1:B:890:LEU:HB3	1:B:983:GLN:HG2	2.00	0.43
1:A:958:SER:O	1:A:962:VAL:HG22	2.19	0.43
1:B:719:ILE:HG13	1:B:720:ARG:N	2.25	0.43
1:B:754:LEU:CD2	1:B:852:THR:HG23	2.44	0.43
1:B:759:ASP:N	1:B:759:ASP:OD1	2.52	0.43
1:B:873:LEU:HD23	1:B:928:PHE:CE2	2.54	0.43
1:B:20:PRO:HG3	1:B:698:VAL:HG23	2.01	0.43
1:B:854:ILE:HD13	1:B:863:VAL:CG1	2.48	0.43
1:A:777:THR:HA	1:A:781:PRO:HA	2.00	0.43
2:C:-9:LYS:HD2	2:C:-9:LYS:HA	1.69	0.43
1:B:26:PHE:CG	1:B:32:VAL:HG22	2.54	0.43
1:A:46:LEU:HG	1:A:54:TYR:HB2	2.01	0.42
1:A:129:VAL:HG21	1:A:231:LEU:HD21	2.01	0.42
1:A:243:LYS:O	1:A:247:ILE:HG12	2.18	0.42
1:A:640:LYS:HE3	1:A:656:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LYS:O	1:A:694:GLU:N	2.50	0.42
1:A:493:THR:HB	1:A:557:LEU:HD23	2.01	0.42
1:A:779:PRO:HB2	1:A:780:LYS:H	1.61	0.42
1:A:623:VAL:HG23	1:A:623:VAL:O	2.19	0.42
1:B:893:VAL:HG11	1:B:979:TYR:HD2	1.82	0.42
1:B:926:LYS:O	1:B:929:LYS:HG3	2.18	0.42
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.90	0.42
1:A:238:ASN:O	1:A:242:THR:HG23	2.19	0.42
1:A:675:LYS:O	1:A:675:LYS:HG2	2.19	0.42
1:B:942:MSE:CE	1:B:952:VAL:HA	2.48	0.42
1:A:30:THR:HG23	3:A:1055:HOH:O	2.19	0.42
1:B:36:VAL:HG21	1:B:57:MSE:HE1	2.01	0.42
1:B:192:GLU:OE2	1:B:207:ARG:NH2	2.51	0.42
1:A:519:VAL:O	1:A:530:GLU:HA	2.20	0.42
1:A:726:VAL:HA	1:A:729:ARG:HG2	2.02	0.42
1:B:30:THR:O	1:B:34:GLU:HG3	2.20	0.42
1:A:45:GLN:HB3	1:A:94:PHE:CE1	2.55	0.42
1:A:942:MSE:CE	1:A:952:VAL:HA	2.47	0.42
1:B:6:PHE:CE2	1:B:321:GLU:HA	2.55	0.42
1:B:498:VAL:O	1:B:521:PRO:HA	2.19	0.42
1:B:873:LEU:O	1:B:873:LEU:HD12	2.20	0.42
1:B:477:ARG:O	1:B:481:ASP:HB2	2.20	0.41
1:B:754:LEU:HD22	1:B:852:THR:CG2	2.47	0.41
1:B:875:LEU:HD23	1:B:875:LEU:HA	1.89	0.41
1:B:885:LYS:HA	1:B:888:ASN:ND2	2.35	0.41
1:A:891:ASN:OD1	1:A:892:LEU:N	2.52	0.41
1:A:44:GLU:HB2	1:A:276:ILE:HG12	2.01	0.41
1:A:873:LEU:HB3	1:A:928:PHE:HZ	1.84	0.41
1:B:18:LEU:HA	1:B:18:LEU:HD23	1.70	0.41
2:C:-17:ASN:O	2:C:-16:LEU:CB	2.68	0.41
1:A:134:VAL:HG23	1:A:135:ASP:OD1	2.20	0.41
1:B:160:THR:HG21	1:B:168:GLU:HA	2.03	0.41
1:B:567:LYS:HE2	1:B:578:TYR:CZ	2.56	0.41
1:A:846:ILE:HD12	1:A:850:LEU:HD11	2.02	0.41
1:B:204:ASP:N	1:B:204:ASP:OD1	2.52	0.41
1:A:964:ASN:HD22	1:A:975:GLU:HG2	1.85	0.41
1:A:146:ASN:HB3	1:A:521:PRO:O	2.20	0.41
1:A:573:GLU:OE1	1:A:573:GLU:N	2.41	0.41
1:B:771:LEU:HD12	1:B:771:LEU:C	2.39	0.41
1:B:971:GLU:CG	1:B:974:LYS:HB2	2.50	0.41
1:A:119:ARG:HB2	1:A:297:GLN:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:OD1	1:A:293:ASP:N	2.51	0.41
1:B:540:ILE:HG23	1:B:540:ILE:HD12	1.78	0.41
1:B:887:LEU:HD23	1:B:887:LEU:O	2.20	0.41
1:B:977:LEU:HD21	1:B:978:ILE:HG12	2.01	0.41
1:A:599:ASP:HA	1:A:617:LYS:HD3	2.02	0.41
1:A:745:SER:O	1:A:749:GLN:HG3	2.20	0.41
1:A:754:LEU:HD21	1:A:851:LEU:HB2	2.03	0.41
1:A:981:THR:O	1:A:985:LEU:HD22	2.20	0.41
1:B:107:GLN:OE1	1:B:109:LYS:HB2	2.20	0.41
1:B:107:GLN:CB	1:B:307:ASN:HB2	2.51	0.41
1:B:974:LYS:HB3	1:B:977:LEU:HD22	2.02	0.41
1:A:129:VAL:HG21	1:A:231:LEU:CD2	2.51	0.41
1:B:24:ARG:HH11	1:B:35:THR:HG21	1.87	0.40
1:B:129:VAL:HG21	1:B:231:LEU:CD2	2.51	0.40
1:A:449:LEU:HD23	1:A:449:LEU:HA	1.92	0.40
1:B:24:ARG:HH11	1:B:35:THR:CG2	2.34	0.40
1:B:127:ARG:HH11	1:B:127:ARG:HD3	1.76	0.40
1:B:57:MSE:O	1:B:60:TYR:HB3	2.21	0.40
1:B:744:ILE:HD12	1:B:783:ILE:HD12	2.04	0.40
1:A:843:ASP:OD1	1:A:963:HIS:HD2	2.05	0.40
1:B:57:MSE:HA	1:B:73:LEU:HD21	2.02	0.40
1:B:873:LEU:HD23	1:B:928:PHE:HE2	1.87	0.40
1:A:56:VAL:HG13	1:A:65:LEU:HD13	2.03	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	947/996 (95%)	879 (93%)	55 (6%)	13 (1%)	11 34
1	B	949/996 (95%)	861 (91%)	70 (7%)	18 (2%)	8 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	11/34 (32%)	6 (54%)	2 (18%)	3 (27%)	0 0
2	D	11/34 (32%)	11 (100%)	0	0	100 100
All	All	1918/2060 (93%)	1757 (92%)	127 (7%)	34 (2%)	8 28

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ILE
1	A	541	ASP
1	A	719	ILE
1	A	779	PRO
1	B	373	PRO
1	B	720	ARG
1	B	973	ASP
2	C	-16	LEU
1	A	163	SER
1	A	164	SER
1	B	18	LEU
1	B	92	GLY
1	B	167	GLU
1	B	717	ALA
1	B	924	TYR
1	B	972	ARG
1	B	975	GLU
2	C	-10	SER
1	A	720	ARG
1	A	973	ASP
1	B	309	ASP
2	C	-17	ASN
1	A	412	ASP
1	A	421	MSE
1	A	778	ASP
1	B	162	ASN
1	B	778	ASP
1	A	422	ASP
1	B	883	ASN
1	B	422	ASP
1	B	881	ASN
1	B	453	VAL
1	A	968	ILE
1	B	779	PRO

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	891/921 (97%)	858 (96%)	33 (4%)	34 68
1	B	888/921 (96%)	854 (96%)	34 (4%)	33 67
2	C	13/28 (46%)	12 (92%)	1 (8%)	13 35
2	D	13/28 (46%)	9 (69%)	4 (31%)	0 0
All	All	1805/1898 (95%)	1733 (96%)	72 (4%)	32 65

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	19	CYS
1	A	73	LEU
1	A	83	ARG
1	A	107[A]	GLN
1	A	107[B]	GLN
1	A	187	ASP
1	A	205	GLU
1	A	236	SER
1	A	238	ASN
1	A	250	ASP
1	A	284	GLN
1	A	449	LEU
1	A	462	SER
1	A	464	ARG
1	A	469	SER
1	A	510	MSE
1	A	562	THR
1	A	582	LEU
1	A	640	LYS
1	A	648	ASP
1	A	650	LYS
1	A	674	ARG
1	A	685	GLU

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Mol	Chain	Res	Type
1	A	704	PRO
1	A	739	TYR
1	A	776	TYR
1	A	789	CYS
1	A	814	THR
1	A	859	ASN
1	A	946	ASP
1	A	954	SER
1	A	981	THR
1	B	14	ARG
1	B	16	THR
1	B	19	CYS
1	B	83	ARG
1	B	105[A]	SER
1	B	105[B]	SER
1	B	107	GLN
1	B	126	ILE
1	B	165	GLU
1	B	186	ASN
1	B	197	THR
1	B	251	LYS
1	B	262	LYS
1	B	297	GLN
1	B	311	LYS
1	B	332	ARG
1	B	397	SER
1	B	420	LYS
1	B	449	LEU
1	B	516	ARG
1	B	564	MSE
1	B	583	ASP
1	B	596	ARG
1	B	662	GLU
1	B	702	VAL
1	B	739	TYR
1	B	759	ASP
1	B	785	LEU
1	B	818	SER
1	B	824	VAL
1	B	869	LEU
1	B	878	PHE
1	B	971	GLU

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Mol	Chain	Res	Type
1	B	977	LEU
2	C	-10	SER
2	D	-20	LYS
2	D	-19	ASP
2	D	-14	LEU
2	D	-13	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	212	GLN
1	A	284	GLN
1	A	430	GLN
1	A	503	ASN
1	A	761	GLN
1	A	766	ASN
1	A	945	GLN
1	A	963	HIS
1	B	130	HIS
1	B	212	GLN
1	B	735	ASN
1	B	888	ASN
1	B	945	GLN
1	B	983	GLN
2	D	-17	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	J9A	D	3	2	12,14,15	1.91	2 (16%)	12,17,19	1.02	0
2	J9A	C	3	2	12,14,15	2.01	1 (8%)	12,17,19	1.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	J9A	D	3	2	-	3/13/16/18	-
2	J9A	C	3	2	-	7/13/16/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	J9A	C06-N07	5.95	1.46	1.33
2	D	3	J9A	C06-N07	5.51	1.45	1.33
2	D	3	J9A	O14-C06	-2.24	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	J9A	C03-C04-C05-C06
2	C	3	J9A	C03-C04-C05-N15
2	C	3	J9A	C02-C03-C04-C05
2	C	3	J9A	N15-C05-C06-O14
2	C	3	J9A	C04-C05-C06-O14
2	D	3	J9A	C02-C03-C04-C05
2	C	3	J9A	O01-C02-C03-C04
2	C	3	J9A	O16-C02-C03-C04
2	D	3	J9A	O01-C02-C03-C04
2	D	3	J9A	O16-C02-C03-C04

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	J9A	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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	939/996 (94%)	-0.42	15 (1%) 72 66	18, 41, 73, 120	0
1	B	935/996 (93%)	-0.29	35 (3%) 41 31	20, 46, 87, 128	0
2	C	15/34 (44%)	0.32	2 (13%) 3 2	31, 47, 109, 116	0
2	D	15/34 (44%)	0.24	1 (6%) 17 10	32, 52, 73, 84	0
All	All	1904/2060 (92%)	-0.34	53 (2%) 53 43	18, 43, 81, 128	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	4	ILE	5.6
1	B	717	ALA	5.0
1	B	626	LYS	4.8
2	D	2	THR	4.3
1	A	166	LEU	4.2
1	B	625	SER	4.1
1	B	423	LEU	4.1
2	C	2	THR	3.9
1	B	972	ARG	3.7
1	B	990	GLU	3.7
1	B	424	GLU	3.4
1	B	986	PHE	3.4
1	B	425	LYS	3.2
1	A	719	ILE	3.1
1	B	64	LEU	3.0
1	B	719	ILE	3.0
1	A	427	SER	3.0
1	A	424	GLU	2.9
1	A	718	PHE	2.9
1	B	975	GLU	2.9
1	B	974	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	985	LEU	2.8
1	A	648	ASP	2.7
1	B	980	TYR	2.7
1	B	443	GLU	2.7
1	A	163	SER	2.6
1	B	881	ASN	2.6
1	B	646	ASN	2.5
1	B	984	ARG	2.5
1	A	858	ASN	2.5
1	B	929	LYS	2.5
1	B	977	LEU	2.5
1	A	425	LYS	2.4
1	B	262	LYS	2.4
1	A	861	TRP	2.4
1	B	206	TYR	2.3
1	B	924	TYR	2.3
1	B	973	ASP	2.3
1	A	646	ASN	2.2
1	B	165	GLU	2.2
1	B	162	ASN	2.2
1	A	694	GLU	2.2
1	B	926	LYS	2.2
1	B	970	ILE	2.2
1	A	164	SER	2.2
1	B	164	SER	2.2
1	B	166	LEU	2.2
1	A	716	ARG	2.2
1	A	717	ALA	2.1
1	B	674	ARG	2.1
1	B	65	LEU	2.1
1	B	880	GLN	2.1
1	B	861	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	J9A	D	3	15/16	0.89	0.19	33,62,82,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	J9A	C	3	15/16	0.90	0.20	41,63,112,116	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.