Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 03:05 am BST

PDB ID	:	3LNN
Title	:	Crystal structure of ZneB from Cupriavidus metallidurans
Authors	:	Lee, J.K.; De Angelis, F.; Miercke, L.J.; Stroud, R.M.; Vandenbussche, G.; Center for Structures of Membrane Proteins (CSMP)
Deposited on	:	2010-02-02
Resolution	:	2.80 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 following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
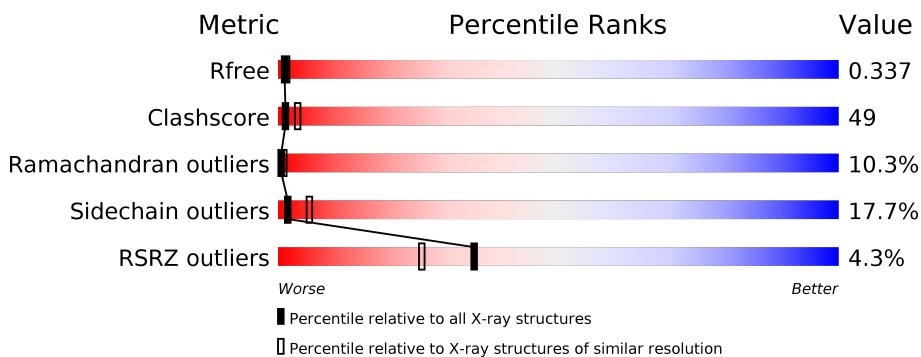
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
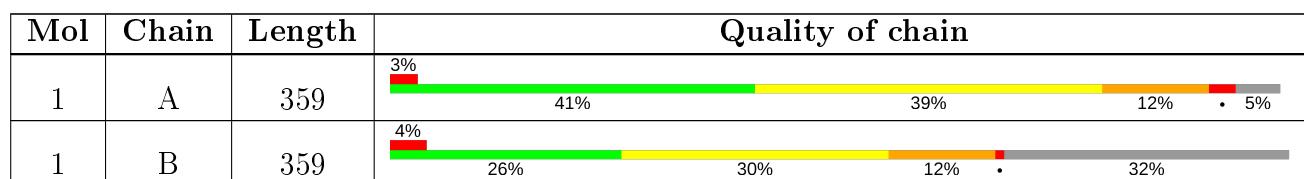
The reported resolution of this entry is 2.80 Å.

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	Percentile Ranks	Value
Rfree		0.337
Clashscore		49
Ramachandran outliers		10.3%
Sidechain outliers		17.7%
RSRZ outliers		4.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	359	3% 41% 39% 12% • 5%
1	B	359	4% 26% 30% 12% • 32%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4361 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 Membrane fusion protein (MFP) heavy metal cation efflux ZneB (CzcB-like).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total 2537	C 1581	N 461	O 487	S 8	0	0	0
1	B	245	Total 1807	C 1120	N 323	O 358	S 6	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q1LCD7
A	351	PRO	-	expression tag	UNP Q1LCD7
A	352	ASP	-	expression tag	UNP Q1LCD7
A	353	LEU	-	expression tag	UNP Q1LCD7
A	354	LEU	-	expression tag	UNP Q1LCD7
A	355	GLU	-	expression tag	UNP Q1LCD7
A	356	VAL	-	expression tag	UNP Q1LCD7
A	357	LEU	-	expression tag	UNP Q1LCD7
A	358	PHE	-	expression tag	UNP Q1LCD7
A	359	GLN	-	expression tag	UNP Q1LCD7
B	1	MET	-	expression tag	UNP Q1LCD7
B	351	PRO	-	expression tag	UNP Q1LCD7
B	352	ASP	-	expression tag	UNP Q1LCD7
B	353	LEU	-	expression tag	UNP Q1LCD7
B	354	LEU	-	expression tag	UNP Q1LCD7
B	355	GLU	-	expression tag	UNP Q1LCD7
B	356	VAL	-	expression tag	UNP Q1LCD7
B	357	LEU	-	expression tag	UNP Q1LCD7
B	358	PHE	-	expression tag	UNP Q1LCD7
B	359	GLN	-	expression tag	UNP Q1LCD7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
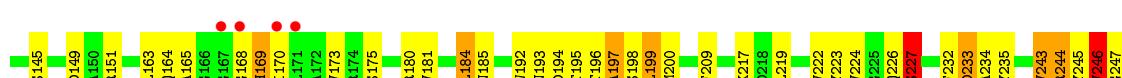
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	11	Total 11	O 11	0	0
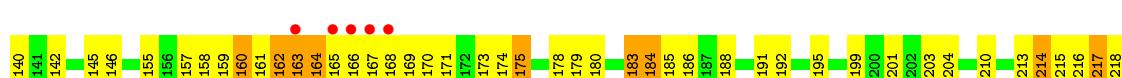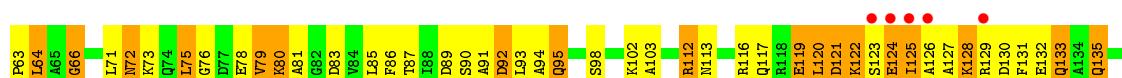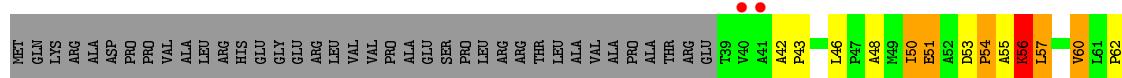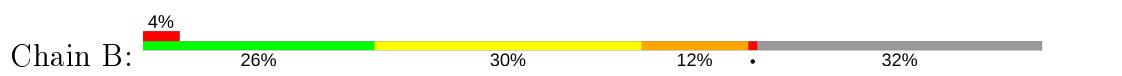
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Membrane fusion protein (MFP) heavy metal cation efflux ZneB (CzcB-like)

• Molecule 1: Membrane fusion protein (MFP) heavy metal cation efflux ZneB (CzcB-like)

VAL VAL PRO MET SER ALA ILE VAL GLN SER GLY PHE THR ARG ALA PHE VAL GLU VAL ALA PRO TRP GLN PHE GLU PRO ARG VAL ILE LYS LEU GLY ALA GLN ILE GLY ASP ARG MET GLU VAL LYS SER GLY LEU SER ALA GLY ASP ARG VAL VAL VAL LYS GLU GLY VAL LEU LEU

ASN ASP PRO ASP LEU LEU GLU VAL LEU PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.11Å 137.11Å 202.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.96 – 2.80 37.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.1 (32.96-2.80) 95.9 (37.38-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.237 , 0.314 0.251 , 0.337	Depositor DCC
R_{free} test set	1188 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	78.6	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.018 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+ 1/2*l,-h+k 0.001 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k- 1/2*l,-h-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4361	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0/2579	0.83	2/3506 (0.1%)
1	B	0.47	0/1834	0.71	1/2493 (0.0%)
All	All	0.50	0/4413	0.79	3/5999 (0.1%)

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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	LYS	N-CA-C	7.18	130.38	111.00
1	B	56	LYS	N-CA-C	-6.99	92.14	111.00
1	A	278	ALA	C-N-CA	5.47	135.38	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ALA	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	2537	0	2501	240	0
1	B	1807	0	1754	190	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
3	B	11	0	0	1	0
All	All	4361	0	4255	424	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 49.

All (424) 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:A:308:VAL:HB	1:A:309:ALA:HB3	1.27	1.11
1:B:93:LEU:HD12	1:B:94:ALA:N	1.66	1.11
1:B:214:ALA:HB1	1:B:215:GLN:HB2	1.25	1.11
1:A:226:GLN:HA	1:A:227:SER:HB2	1.34	1.09
1:A:319:LYS:HA	1:A:320:LEU:HB2	1.26	1.09
1:A:55:ALA:HA	1:A:57:LEU:H	1.13	1.07
1:B:93:LEU:HD12	1:B:94:ALA:H	1.12	1.06
1:A:323:GLN:O	1:A:324:ILE:HG13	1.54	1.05
1:A:245:TYR:HA	1:A:246:VAL:HG23	1.38	1.04
1:B:219:LEU:HD21	1:B:257:THR:HG21	1.39	1.04
1:B:117:GLN:OE1	1:B:131:PHE:HA	1.56	1.04
1:A:292:MET:HE1	1:A:328:MET:HG2	1.42	1.02
1:B:93:LEU:CD1	1:B:169:HIS:HA	1.88	1.02
1:A:104:ARG:HG3	1:A:104:ARG:HH11	1.22	1.02
1:B:183:ASP:HB2	1:B:201:THR:HB	1.42	1.02
1:B:93:LEU:HD13	1:B:169:HIS:CA	1.92	1.00
1:A:246:VAL:HG12	1:A:247:GLY:N	1.77	0.99
1:A:292:MET:CE	1:A:328:MET:HG2	1.93	0.97
1:A:103:ALA:HB1	1:A:145:SER:HA	1.46	0.97
1:A:217:LYS:HE3	1:A:322:ALA:HA	1.47	0.96
1:A:343:LYS:CB	1:A:344:GLU:HA	1.96	0.95
1:A:194:ASP:HB3	1:A:197:ALA:HB2	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:SER:HB3	1:B:283:GLN:HA	1.44	0.94
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.30	0.94
1:A:195:THR:HA	1:A:196:THR:C	1.84	0.94
1:B:93:LEU:HD13	1:B:169:HIS:HA	0.97	0.94
1:B:142:ALA:O	1:B:146:GLN:HG3	1.69	0.93
1:B:174:ARG:O	1:B:175:SER:HB3	1.67	0.92
1:A:301:TYR:HA	1:A:302:THR:HG22	1.52	0.91
1:A:323:GLN:HB3	1:A:328:MET:HE2	1.53	0.91
1:A:344:GLU:HG2	1:A:345:GLY:H	1.34	0.90
1:B:282:SER:CB	1:B:283:GLN:HA	2.01	0.90
1:B:85:LEU:HD11	1:B:175:SER:HB2	1.53	0.88
1:A:226:GLN:CA	1:A:227:SER:HB2	2.04	0.88
1:B:214:ALA:HB1	1:B:215:GLN:CB	2.04	0.88
1:A:316:ARG:CG	1:A:316:ARG:HH11	1.86	0.87
1:B:199:LEU:H	1:B:199:LEU:HD23	1.40	0.86
1:B:267:ASP:OD1	1:B:269:ARG:HG3	1.74	0.86
1:A:278:ALA:HA	1:A:279:THR:OG1	1.74	0.86
1:B:223:TYR:CZ	1:B:226:GLN:HB3	2.10	0.86
1:B:265:ASN:N	1:B:266:PRO:HD2	1.91	0.85
1:A:246:VAL:HG12	1:A:247:GLY:H	1.40	0.83
1:A:55:ALA:HA	1:A:57:LEU:N	1.91	0.83
1:A:195:THR:HA	1:A:196:THR:O	1.79	0.82
1:B:265:ASN:H	1:B:266:PRO:CD	1.92	0.82
1:A:21:PRO:HA	1:A:22:ALA:HB3	1.62	0.82
1:A:308:VAL:HG23	1:A:312:GLN:O	1.80	0.82
1:B:215:GLN:HB3	1:B:218:ASP:OD2	1.79	0.82
1:A:320:LEU:H	1:A:331:LYS:HG2	1.44	0.81
1:B:219:LEU:CD2	1:B:257:THR:HG21	2.11	0.81
1:B:265:ASN:H	1:B:266:PRO:HD2	1.46	0.80
1:A:319:LYS:CA	1:A:320:LEU:HB2	2.11	0.79
1:A:85:LEU:HD11	1:A:175:SER:HB2	1.65	0.79
1:B:234:ALA:O	1:B:235:TYR:HB2	1.82	0.78
1:A:245:TYR:HA	1:A:246:VAL:CG2	2.12	0.78
1:B:124:GLU:HG3	1:B:125:ILE:HG23	1.66	0.77
1:A:296:VAL:HG21	1:A:347:LEU:HD23	1.64	0.77
1:B:160:GLY:HA2	1:B:171:LEU:HD21	1.66	0.76
1:A:37:ARG:HG2	1:A:286:GLU:HG3	1.67	0.76
1:B:98:SER:O	1:B:102:LYS:HG2	1.85	0.76
1:B:214:ALA:CB	1:B:215:GLN:HB2	2.12	0.75
1:A:297:GLN:HA	1:A:302:THR:H	1.50	0.74
1:A:324:ILE:HD12	1:A:324:ILE:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:HD12	1:A:289:VAL:N	2.02	0.74
1:A:300:PHE:O	1:A:301:TYR:CG	2.41	0.74
1:A:300:PHE:O	1:A:301:TYR:CD1	2.41	0.73
1:A:319:LYS:HA	1:A:320:LEU:CB	2.14	0.73
1:A:342:VAL:N	1:A:343:LYS:HA	2.02	0.73
1:B:165:ALA:HB1	1:B:166:GLY:HA2	1.70	0.73
1:B:244:ARG:HB3	1:B:244:ARG:HH11	1.51	0.73
1:A:21:PRO:HA	1:A:22:ALA:CB	2.17	0.73
1:A:234:ALA:HB2	1:B:217:LYS:HA	1.70	0.72
1:A:197:ALA:O	1:A:198:SER:HB3	1.89	0.72
1:B:122:LYS:HA	1:B:124:GLU:N	2.04	0.72
1:A:76:GLY:O	1:A:180:ARG:NH1	2.23	0.72
1:A:18:LEU:HD13	1:A:346:VAL:HG22	1.73	0.71
1:B:282:SER:HB3	1:B:283:GLN:CA	2.19	0.71
1:A:116:ARG:O	1:A:117:GLN:HG3	1.91	0.71
1:B:53:ASP:O	1:B:56:LYS:HB2	1.91	0.71
1:A:246:VAL:CG1	1:A:247:GLY:N	2.48	0.70
1:B:199:LEU:HD23	1:B:199:LEU:N	2.06	0.70
1:B:221:HIS:CD2	1:B:283:GLN:H	2.09	0.70
1:B:214:ALA:N	1:B:256:THR:HB	2.06	0.70
1:B:117:GLN:HG2	1:B:131:PHE:HD2	1.56	0.70
1:B:222:VAL:HA	1:B:226:GLN:HE22	1.57	0.69
1:B:265:ASN:N	1:B:266:PRO:CD	2.53	0.69
1:A:21:PRO:CA	1:A:22:ALA:HB3	2.22	0.69
1:B:79:VAL:HA	1:B:80:LYS:CB	2.22	0.69
1:B:221:HIS:HD2	1:B:283:GLN:H	1.40	0.69
1:A:245:TYR:CG	1:A:246:VAL:HB	2.26	0.69
1:A:91:ALA:N	1:A:92:ASP:HB2	2.08	0.69
1:B:213:ASN:O	1:B:214:ALA:HB3	1.93	0.69
1:B:90:SER:HB3	1:B:93:LEU:HG	1.75	0.69
1:A:316:ARG:NH1	1:A:316:ARG:HG3	2.05	0.68
1:A:301:TYR:HA	1:A:302:THR:CG2	2.24	0.68
1:B:219:LEU:HD21	1:B:257:THR:CG2	2.21	0.67
1:A:104:ARG:CG	1:A:104:ARG:HH11	2.03	0.67
1:B:192:TRP:CH2	1:B:199:LEU:HB3	2.29	0.67
1:B:226:GLN:H	1:B:243:VAL:HG22	1.60	0.67
1:A:343:LYS:CB	1:A:344:GLU:CA	2.73	0.67
1:A:344:GLU:N	1:A:344:GLU:OE1	2.28	0.66
1:A:45:ASN:ND2	1:A:277:GLN:OE1	2.29	0.66
1:A:344:GLU:CG	1:A:345:GLY:H	2.08	0.66
1:A:16:GLU:C	1:A:16:GLU:CD	2.55	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HG22	1:A:196:THR:HA	1.78	0.65
1:B:93:LEU:CD1	1:B:94:ALA:N	2.53	0.65
1:B:122:LYS:HA	1:B:124:GLU:H	1.61	0.65
1:A:244:ARG:HB3	1:A:244:ARG:HH11	1.62	0.65
1:B:113:ASN:O	1:B:116:ARG:HB2	1.97	0.65
1:B:183:ASP:HB2	1:B:201:THR:CB	2.23	0.65
1:B:223:TYR:CE2	1:B:226:GLN:HB3	2.32	0.65
1:A:32:VAL:HG13	1:A:340:VAL:O	1.96	0.65
1:B:261:MET:HE2	1:B:263:PHE:HE2	1.62	0.65
1:A:341:VAL:HG12	1:A:343:LYS:O	1.97	0.65
1:A:308:VAL:CB	1:A:309:ALA:HB3	2.17	0.64
1:A:274:MET:CE	1:B:219:LEU:HD13	2.28	0.64
1:A:184:LEU:O	1:A:199:LEU:O	2.16	0.64
1:B:122:LYS:CA	1:B:124:GLU:H	2.10	0.64
1:A:305:PHE:O	1:A:341:VAL:HG23	1.96	0.64
1:A:341:VAL:CG1	1:A:343:LYS:O	2.45	0.64
1:A:249:ILE:HD12	1:A:250:LEU:H	1.63	0.64
1:A:104:ARG:NH1	1:A:104:ARG:HG3	2.02	0.63
1:A:103:ALA:HB1	1:A:145:SER:CA	2.26	0.63
1:A:310:PRO:O	1:A:311:TRP:HB2	1.98	0.63
1:B:160:GLY:CA	1:B:171:LEU:HD21	2.28	0.63
1:A:46:LEU:N	1:A:278:ALA:O	2.28	0.62
1:B:222:VAL:HA	1:B:226:GLN:NE2	2.13	0.62
1:A:199:LEU:HD23	1:A:199:LEU:N	2.13	0.62
1:B:117:GLN:HG2	1:B:131:PHE:CD2	2.35	0.62
1:A:170:ILE:HD12	1:A:170:ILE:O	1.99	0.62
1:A:331:LYS:O	1:A:332:SER:HB3	1.99	0.62
1:A:344:GLU:HG2	1:A:345:GLY:N	2.10	0.62
1:B:79:VAL:HG23	1:B:80:LYS:CB	2.28	0.62
1:A:57:LEU:O	1:A:57:LEU:HD23	2.00	0.62
1:B:125:ILE:HG13	1:B:126:ALA:N	2.14	0.62
1:B:46:LEU:HD12	1:B:280:PHE:CE2	2.35	0.62
1:A:301:TYR:CA	1:A:302:THR:HG22	2.29	0.61
1:A:323:GLN:HB3	1:A:328:MET:CE	2.29	0.61
1:A:292:MET:HE2	1:A:328:MET:HG2	1.81	0.61
1:B:246:VAL:HG13	1:B:247:GLY:N	2.16	0.60
1:B:50:ILE:HD11	1:B:272:PRO:N	2.16	0.60
1:B:64:LEU:HD23	1:B:158:LYS:HE2	1.84	0.60
1:B:92:ASP:OD1	1:B:92:ASP:N	2.33	0.60
1:A:219:LEU:CD1	1:A:257:THR:HG21	2.31	0.60
1:A:278:ALA:CA	1:A:279:THR:OG1	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:O	1:A:302:THR:HG23	2.02	0.60
1:B:120:LEU:O	1:B:122:LYS:N	2.34	0.60
1:B:103:ALA:HB1	1:B:145:SER:HA	1.84	0.60
1:B:128:LYS:O	1:B:128:LYS:HD2	2.03	0.59
1:B:214:ALA:CA	1:B:256:THR:HB	2.32	0.59
1:A:15:GLY:O	1:A:16:GLU:CB	2.51	0.59
1:B:57:LEU:HB2	1:B:203:ALA:HB2	1.84	0.59
1:A:300:PHE:HD2	1:A:300:PHE:H	1.49	0.59
1:A:181:VAL:HG22	1:A:200:MET:CE	2.32	0.59
1:B:66:GLY:HA2	1:B:192:TRP:O	2.02	0.59
1:A:288:ILE:HD12	1:A:289:VAL:H	1.67	0.59
1:A:120:LEU:O	1:A:126:ALA:HA	2.02	0.59
1:A:74:GLN:HB2	1:A:77:ASP:OD2	2.03	0.59
1:A:265:ASN:OD1	1:A:270:LEU:HB2	2.03	0.58
1:A:192:TRP:HE1	1:A:197:ALA:HB3	1.68	0.58
1:A:194:ASP:OD1	1:A:195:THR:N	2.36	0.58
1:A:217:LYS:HD2	1:A:321:GLY:HA3	1.84	0.58
1:A:32:VAL:HG11	1:A:339:ARG:HB3	1.85	0.58
1:A:269:ARG:HH11	1:A:269:ARG:HG3	1.68	0.58
1:A:40:VAL:HG23	1:A:285:HIS:CE1	2.39	0.57
1:A:297:GLN:HA	1:A:302:THR:N	2.19	0.57
1:A:17:ARG:NH1	1:A:312:GLN:OE1	2.34	0.57
1:B:79:VAL:CA	1:B:80:LYS:CB	2.82	0.57
1:A:264:ASP:OD2	1:A:266:PRO:HG3	2.05	0.57
1:B:117:GLN:CD	1:B:131:PHE:HA	2.23	0.57
1:A:347:LEU:O	1:A:347:LEU:HG	2.05	0.57
1:B:225:GLY:HA2	1:B:243:VAL:HG23	1.85	0.57
1:A:226:GLN:HA	1:A:227:SER:CB	2.23	0.57
1:B:75:LEU:HD12	1:B:76:GLY:N	2.20	0.57
1:A:192:TRP:CE2	1:A:199:LEU:HD22	2.38	0.56
1:A:40:VAL:CG2	1:A:285:HIS:NE2	2.67	0.56
1:B:265:ASN:O	1:B:266:PRO:C	2.42	0.56
1:A:195:THR:CA	1:A:196:THR:C	2.65	0.56
1:A:244:ARG:CB	1:A:244:ARG:HH11	2.18	0.56
1:A:271:ARG:HG3	1:A:274:MET:HE3	1.86	0.56
1:B:169:HIS:C	1:B:170:ILE:HD12	2.26	0.56
1:A:274:MET:HE1	1:B:219:LEU:HD13	1.88	0.56
1:A:251:ASP:O	1:A:253:ASP:N	2.38	0.56
1:B:265:ASN:HD22	1:B:270:LEU:HB2	1.70	0.55
1:A:130:ASP:HA	1:A:132:GLU:OE1	2.07	0.55
1:A:91:ALA:H	1:A:92:ASP:HB2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:O	1:B:171:LEU:HD12	2.05	0.55
1:B:48:ALA:HB1	1:B:210:VAL:HG12	1.89	0.55
1:B:259:VAL:O	1:B:259:VAL:HG12	2.06	0.55
1:B:124:GLU:HA	1:B:125:ILE:HG22	1.87	0.55
1:A:192:TRP:HE1	1:A:197:ALA:CB	2.20	0.55
1:A:300:PHE:HD2	1:A:300:PHE:N	2.04	0.55
1:A:245:TYR:HA	1:A:246:VAL:CB	2.35	0.54
1:A:123:SER:O	1:A:124:GLU:HB2	2.07	0.54
1:B:50:ILE:C	1:B:51:GLU:HG3	2.26	0.54
1:A:32:VAL:HG12	1:A:33:ALA:N	2.23	0.54
1:B:214:ALA:HB1	1:B:215:GLN:OE1	2.08	0.54
1:B:244:ARG:CB	1:B:244:ARG:HH11	2.20	0.54
1:A:195:THR:HG23	1:A:196:THR:O	2.08	0.54
1:B:236:ASP:O	1:B:237:ASP:OD1	2.26	0.54
1:A:192:TRP:CE2	1:A:199:LEU:CD2	2.91	0.54
1:A:295:ILE:HD12	1:A:296:VAL:N	2.23	0.54
1:A:69:VAL:HB	1:A:87:THR:OG1	2.06	0.54
1:A:343:LYS:H	1:A:344:GLU:HB3	1.73	0.54
1:B:267:ASP:OD1	1:B:267:ASP:C	2.47	0.54
1:A:223:TYR:CZ	1:A:226:GLN:HG2	2.43	0.53
1:B:57:LEU:HD13	1:B:57:LEU:O	2.06	0.53
1:A:269:ARG:NH1	1:A:269:ARG:HG3	2.22	0.53
1:A:217:LYS:CE	1:A:322:ALA:HA	2.31	0.53
1:B:64:LEU:HD23	1:B:158:LYS:CE	2.38	0.53
1:B:246:VAL:HG13	1:B:247:GLY:O	2.09	0.53
1:A:185:ASN:ND2	1:A:185:ASN:O	2.39	0.53
1:B:129:ARG:O	1:B:131:PHE:N	2.41	0.53
1:A:245:TYR:CD1	1:A:246:VAL:HB	2.44	0.53
1:B:122:LYS:N	1:B:123:SER:HB2	2.24	0.53
1:B:258:LYS:O	1:B:259:VAL:HG23	2.08	0.53
1:B:93:LEU:HD11	1:B:169:HIS:O	2.08	0.53
1:A:24:SER:OG	1:A:26:LEU:HD22	2.09	0.53
1:A:320:LEU:N	1:A:331:LYS:HG2	2.20	0.53
1:A:300:PHE:CD2	1:A:300:PHE:N	2.77	0.53
1:B:124:GLU:HA	1:B:125:ILE:CG2	2.39	0.52
1:A:61:LEU:HD23	1:A:198:SER:HB2	1.91	0.52
1:A:319:LYS:CA	1:A:320:LEU:CB	2.83	0.52
1:B:246:VAL:O	1:B:258:LYS:O	2.27	0.52
1:B:75:LEU:HD12	1:B:76:GLY:H	1.75	0.52
1:B:78:GLU:HG3	1:B:180:ARG:CZ	2.40	0.52
1:B:165:ALA:HA	1:B:166:GLY:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HA	1:A:29:THR:OG1	2.10	0.52
1:B:214:ALA:HA	1:B:256:THR:HB	1.91	0.52
1:A:18:LEU:CD1	1:A:346:VAL:HG22	2.40	0.52
1:B:168:GLY:O	1:B:169:HIS:HB3	2.09	0.52
1:A:54:PRO:O	1:A:55:ALA:HB2	2.10	0.52
1:A:224:VAL:HG21	1:A:246:VAL:HG22	1.91	0.52
1:A:24:SER:OG	1:A:26:LEU:CD2	2.57	0.52
1:A:68:ILE:HG21	1:A:71:LEU:HD11	1.91	0.52
1:A:274:MET:HE2	1:B:219:LEU:HD13	1.91	0.51
1:B:215:GLN:O	1:B:216:GLU:C	2.49	0.51
1:A:128:LYS:HD2	1:A:129:ARG:H	1.75	0.51
1:B:112:ARG:NH1	1:B:116:ARG:HG2	2.24	0.51
1:B:224:VAL:HA	1:B:243:VAL:HG23	1.92	0.51
1:B:131:PHE:O	1:B:133:GLN:N	2.43	0.51
1:B:85:LEU:CD1	1:B:175:SER:HB2	2.33	0.51
1:A:261:MET:HG3	1:A:263:PHE:HE2	1.75	0.51
1:A:267:ASP:H	1:A:268:GLY:HA2	1.75	0.51
1:A:308:VAL:HB	1:A:309:ALA:CB	2.20	0.51
1:B:112:ARG:HH12	1:B:116:ARG:HG2	1.74	0.51
1:B:56:LYS:HD2	1:B:204:ASP:HB3	1.91	0.51
1:A:114:LEU:CD1	1:A:134:ALA:HB1	2.41	0.51
1:A:15:GLY:O	1:A:16:GLU:HB2	2.11	0.51
1:A:296:VAL:HG13	1:A:303:ARG:O	2.11	0.50
1:A:316:ARG:CG	1:A:316:ARG:NH1	2.57	0.50
1:A:333:GLY:HA2	1:A:334:LEU:O	2.11	0.50
1:A:107:MET:HG3	1:A:142:ALA:HA	1.92	0.50
1:A:235:TYR:CZ	1:A:269:ARG:HB2	2.47	0.50
1:A:295:ILE:HD12	1:A:296:VAL:H	1.76	0.50
1:B:135:GLN:OE1	1:B:135:GLN:O	2.29	0.50
1:B:264:ASP:HB3	1:B:266:PRO:HD2	1.93	0.50
1:A:70:SER:C	1:A:71:LEU:HD12	2.32	0.50
1:A:26:LEU:H	1:A:26:LEU:CD2	2.25	0.49
1:B:275:PHE:CG	1:B:276:ALA:N	2.80	0.49
1:B:213:ASN:O	1:B:214:ALA:CB	2.58	0.49
1:A:296:VAL:O	1:A:302:THR:HA	2.13	0.49
1:A:302:THR:O	1:A:302:THR:CG2	2.60	0.49
1:A:104:ARG:NH1	1:A:149:ASP:OD1	2.45	0.49
1:A:164:GLN:OE1	1:A:165:ALA:N	2.44	0.49
1:A:235:TYR:CE2	1:A:269:ARG:HB2	2.47	0.49
1:B:79:VAL:O	1:B:179:GLY:O	2.31	0.49
1:A:307:GLU:OE1	1:A:310:PRO:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:VAL:HG23	1:B:243:VAL:O	2.12	0.49
1:B:63:PRO:O	1:B:64:LEU:CB	2.60	0.49
1:A:26:LEU:N	1:A:26:LEU:CD2	2.76	0.49
1:B:131:PHE:C	1:B:133:GLN:H	2.16	0.49
1:A:57:LEU:C	1:A:57:LEU:HD23	2.33	0.48
1:A:81:ALA:HA	1:A:82:GLY:HA2	1.52	0.48
1:B:157:ALA:C	1:B:159:GLY:H	2.15	0.48
1:B:90:SER:HB3	1:B:93:LEU:CG	2.42	0.48
1:B:215:GLN:O	1:B:218:ASP:N	2.42	0.48
1:A:199:LEU:N	1:A:199:LEU:CD2	2.76	0.48
1:A:100:ALA:HB1	1:A:104:ARG:NH1	2.29	0.48
1:A:24:SER:OG	1:A:25:PRO:HD2	2.12	0.48
1:A:271:ARG:HH11	1:A:274:MET:CE	2.26	0.48
1:A:50:ILE:HG22	1:A:272:PRO:HA	1.96	0.48
1:B:116:ARG:O	1:B:119:GLU:HB3	2.14	0.48
1:A:224:VAL:HA	1:A:243:VAL:HG23	1.96	0.48
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.64	0.48
1:B:90:SER:HB3	1:B:93:LEU:CD2	2.43	0.48
1:A:93:LEU:HD23	1:A:169:HIS:HB3	1.95	0.48
1:A:16:GLU:OE1	1:A:17:ARG:N	2.46	0.48
1:A:309:ALA:HB1	1:A:312:GLN:CD	2.33	0.48
1:B:163:LEU:H	1:B:163:LEU:HG	1.34	0.48
1:B:90:SER:CB	1:B:93:LEU:HG	2.41	0.48
1:A:26:LEU:HD22	1:A:26:LEU:H	1.78	0.48
1:B:131:PHE:C	1:B:133:GLN:N	2.64	0.48
1:A:24:SER:OG	1:A:25:PRO:CD	2.62	0.48
1:A:347:LEU:O	1:A:347:LEU:CG	2.61	0.48
1:B:78:GLU:HG3	1:B:180:ARG:NH1	2.29	0.47
1:B:90:SER:O	1:B:93:LEU:CD1	2.62	0.47
1:A:112:ARG:O	1:A:116:ARG:HG2	2.14	0.47
1:A:194:ASP:CB	1:A:197:ALA:HB2	2.31	0.47
1:B:261:MET:HE2	1:B:263:PHE:CE2	2.47	0.47
1:A:129:ARG:O	1:A:131:PHE:N	2.47	0.47
1:A:192:TRP:NE1	1:A:197:ALA:CB	2.77	0.47
1:B:258:LYS:HG3	3:B:369:HOH:O	2.13	0.47
1:B:63:PRO:O	1:B:64:LEU:HB2	2.15	0.47
1:B:87:THR:HA	1:B:171:LEU:O	2.15	0.47
1:B:50:ILE:HD11	1:B:271:ARG:C	2.36	0.47
1:B:214:ALA:H	1:B:256:THR:HB	1.79	0.47
1:A:129:ARG:HD2	1:A:132:GLU:OE2	2.16	0.46
1:A:300:PHE:C	1:A:301:TYR:CG	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:HG11	1:A:343:LYS:O	2.15	0.46
1:A:62:PRO:HG3	1:A:192:TRP:CD1	2.50	0.46
1:A:20:VAL:O	1:A:27:ARG:NH1	2.49	0.46
1:B:246:VAL:CG1	1:B:247:GLY:N	2.77	0.46
1:A:196:THR:O	1:A:197:ALA:HB3	2.16	0.46
1:B:86:PHE:CZ	1:B:173:VAL:HG11	2.51	0.46
1:B:184:LEU:O	1:B:185:ASN:OD1	2.34	0.46
1:A:192:TRP:NE1	1:A:197:ALA:HB1	2.31	0.46
1:B:214:ALA:HB1	1:B:215:GLN:CA	2.46	0.46
1:A:302:THR:HG23	1:A:318:ILE:O	2.16	0.46
1:A:102:LYS:O	1:A:103:ALA:C	2.55	0.45
1:B:223:TYR:H	1:B:226:GLN:HE21	1.64	0.45
1:A:104:ARG:CZ	1:A:149:ASP:OD1	2.64	0.45
1:B:50:ILE:CD1	1:B:272:PRO:HA	2.47	0.45
1:A:251:ASP:O	1:A:251:ASP:OD1	2.35	0.45
1:B:76:GLY:O	1:B:180:ARG:NH1	2.46	0.45
1:A:219:LEU:HD11	1:A:257:THR:HG21	1.97	0.45
1:B:223:TYR:H	1:B:226:GLN:NE2	2.15	0.45
1:B:50:ILE:HD11	1:B:272:PRO:CA	2.46	0.45
1:B:124:GLU:CG	1:B:125:ILE:HG23	2.41	0.45
1:A:50:ILE:HD12	1:A:274:MET:HB2	1.99	0.45
1:A:129:ARG:HG3	1:A:132:GLU:CD	2.38	0.44
1:A:295:ILE:HD13	1:A:318:ILE:HD11	1.98	0.44
1:B:60:VAL:HG21	1:B:86:PHE:HE1	1.83	0.44
1:B:62:PRO:HD3	1:B:199:LEU:CD2	2.47	0.44
1:B:265:ASN:O	1:B:267:ASP:N	2.51	0.44
1:A:104:ARG:NH1	1:A:104:ARG:CG	2.69	0.44
1:B:90:SER:O	1:B:93:LEU:HD11	2.17	0.44
1:A:45:ASN:HA	1:A:279:THR:H	1.82	0.44
1:B:226:GLN:N	1:B:243:VAL:HG22	2.31	0.44
1:A:114:LEU:HD13	1:A:134:ALA:HB1	2.00	0.44
1:A:181:VAL:HG22	1:A:200:MET:HE1	2.00	0.43
1:A:71:LEU:HD12	1:A:71:LEU:N	2.33	0.43
1:B:125:ILE:CG1	1:B:126:ALA:N	2.78	0.43
1:B:91:ALA:O	1:B:95:GLN:HB2	2.18	0.43
1:A:290:VAL:HG22	1:A:330:VAL:HG23	1.99	0.43
1:A:292:MET:HE2	1:A:328:MET:HB2	1.98	0.43
1:B:57:LEU:CB	1:B:203:ALA:HB2	2.48	0.43
1:A:184:LEU:O	1:A:185:ASN:CG	2.56	0.43
1:A:192:TRP:CE2	1:A:197:ALA:HB1	2.54	0.43
1:A:217:LYS:HZ1	1:A:323:GLN:CG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ARG:HD2	1:B:112:ARG:HA	1.52	0.43
1:A:61:LEU:HD22	1:A:196:THR:CA	2.49	0.43
1:A:86:PHE:CE2	1:A:173:VAL:HG21	2.54	0.43
1:A:331:LYS:O	1:A:332:SER:CB	2.66	0.43
1:B:122:LYS:HA	1:B:123:SER:C	2.38	0.43
1:B:186:ALA:CB	1:B:199:LEU:HB2	2.48	0.43
1:B:199:LEU:CD2	1:B:199:LEU:N	2.79	0.43
1:B:234:ALA:O	1:B:235:TYR:CB	2.59	0.43
1:B:251:ASP:O	1:B:253:ASP:N	2.52	0.43
1:A:30:LEU:HD22	1:A:343:LYS:O	2.19	0.43
1:B:60:VAL:CG2	1:B:86:PHE:HE1	2.31	0.43
1:A:323:GLN:O	1:A:324:ILE:CG1	2.46	0.43
1:B:102:LYS:O	1:B:103:ALA:C	2.55	0.43
1:B:120:LEU:O	1:B:121:ASP:C	2.57	0.43
1:A:164:GLN:OE1	1:A:164:GLN:HA	2.18	0.42
1:A:224:VAL:HA	1:A:243:VAL:CG2	2.49	0.42
1:B:254:THR:O	1:B:255:ARG:HB2	2.19	0.42
1:B:225:GLY:HA2	1:B:243:VAL:CG2	2.48	0.42
1:A:272:PRO:HD2	1:B:248:GLN:O	2.19	0.42
1:A:249:ILE:HD12	1:A:250:LEU:N	2.32	0.42
1:A:233:ASP:HA	1:A:234:ALA:HA	1.66	0.42
1:A:293:SER:OG	1:A:342:VAL:HG12	2.20	0.42
1:A:226:GLN:CB	1:A:227:SER:HB2	2.49	0.42
1:B:233:ASP:HA	1:B:234:ALA:HA	1.45	0.42
1:A:209:PHE:CE1	1:A:262:VAL:HG22	2.55	0.42
1:A:35:ALA:HB1	1:A:288:ILE:HD13	2.01	0.42
1:B:165:ALA:HA	1:B:167:GLY:N	2.35	0.42
1:B:42:ALA:HA	1:B:43:PRO:HD2	1.87	0.42
1:B:83:ASP:O	1:B:174:ARG:O	2.37	0.42
1:A:267:ASP:N	1:A:268:GLY:HA2	2.33	0.42
1:A:109:MET:HE2	1:B:140:GLN:HA	2.02	0.42
1:B:271:ARG:HA	1:B:272:PRO:HD3	1.91	0.42
1:B:72:ASN:OD1	1:B:72:ASN:N	2.52	0.42
1:A:324:ILE:HA	1:A:325:GLY:HA2	1.57	0.41
1:A:94:ALA:O	1:A:95:GLN:C	2.57	0.41
1:B:89:ASP:OD1	1:B:169:HIS:HE1	2.03	0.41
1:A:117:GLN:OE1	1:A:134:ALA:HB2	2.21	0.41
1:B:50:ILE:HD11	1:B:272:PRO:HA	2.01	0.41
1:B:54:PRO:HA	1:B:55:ALA:HA	1.58	0.41
1:A:296:VAL:CG2	1:A:297:GLN:N	2.83	0.41
1:B:126:ALA:HA	1:B:127:ALA:HA	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:O	1:A:243:VAL:CG2	2.68	0.41
1:A:320:LEU:HA	1:A:320:LEU:HD12	1.86	0.41
1:B:237:ASP:HA	1:B:238:PRO:HD3	1.67	0.41
1:B:223:TYR:O	1:B:243:VAL:CG2	2.69	0.41
1:B:63:PRO:O	1:B:64:LEU:HG	2.21	0.41
1:A:124:GLU:O	1:A:125:ILE:HG13	2.21	0.41
1:A:100:ALA:O	1:A:104:ARG:NH1	2.54	0.41
1:A:114:LEU:HD13	1:A:134:ALA:C	2.41	0.41
1:A:195:THR:CG2	1:A:196:THR:HA	2.48	0.41
1:A:271:ARG:HB2	1:A:274:MET:HE2	2.02	0.41
1:B:236:ASP:O	1:B:237:ASP:CG	2.59	0.41
1:A:10:ALA:HA	1:A:11:LEU:CB	2.51	0.41
1:A:334:LEU:HA	1:A:334:LEU:HD12	1.87	0.41
1:B:270:LEU:N	1:B:270:LEU:CD1	2.84	0.41
1:B:163:LEU:O	1:B:164:GLN:HB2	2.20	0.41
1:B:62:PRO:O	1:B:195:THR:HG22	2.21	0.41
1:B:254:THR:HB	1:B:256:THR:HG23	2.03	0.41
1:B:50:ILE:C	1:B:50:ILE:HD12	2.41	0.41
1:B:50:ILE:CG1	1:B:271:ARG:O	2.69	0.41
1:A:114:LEU:HD21	1:A:135:GLN:OE1	2.21	0.41
1:A:244:ARG:CG	1:A:244:ARG:HH11	2.32	0.41
1:B:63:PRO:O	1:B:63:PRO:HG2	2.21	0.41
1:A:243:VAL:HA	1:A:261:MET:HB3	2.03	0.40
1:A:114:LEU:HD12	1:A:134:ALA:HB1	2.03	0.40
1:A:122:LYS:O	1:A:123:SER:C	2.59	0.40
1:A:163:LEU:HG	1:A:164:GLN:N	2.36	0.40
1:B:121:ASP:CG	1:B:121:ASP:O	2.58	0.40
1:B:66:GLY:HA3	1:B:191:TYR:HE1	1.86	0.40
1:B:50:ILE:HG12	1:B:271:ARG:O	2.21	0.40
1:B:93:LEU:H	1:B:93:LEU:HG	1.74	0.40
1:A:38:GLU:OE1	1:A:327:ARG:NH2	2.50	0.40
1:A:98:SER:O	1:A:101:ALA:HB3	2.22	0.40
1:A:344:GLU:CG	1:A:345:GLY:N	2.77	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	339/359 (94%)	266 (78%)	39 (12%)	34 (10%)	0	1
1	B	243/359 (68%)	192 (79%)	25 (10%)	26 (11%)	0	1
All	All	582/718 (81%)	458 (79%)	64 (11%)	60 (10%)	0	1

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	23	GLU
1	A	56	LYS
1	A	122	LYS
1	A	123	SER
1	A	227	SER
1	A	233	ASP
1	A	246	VAL
1	A	320	LEU
1	A	332	SER
1	B	56	LYS
1	B	80	LYS
1	B	81	ALA
1	B	121	ASP
1	B	122	LYS
1	B	130	ASP
1	B	235	TYR
1	B	236	ASP
1	B	259	VAL
1	B	265	ASN
1	B	266	PRO
1	A	94	ALA
1	A	95	GLN
1	A	130	ASP
1	A	279	THR

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Mol	Chain	Res	Type
1	A	302	THR
1	B	73	LYS
1	B	119	GLU
1	B	125	ILE
1	A	73	LYS
1	A	96	ALA
1	A	197	ALA
1	A	252	ALA
1	A	301	TYR
1	A	309	ALA
1	A	334	LEU
1	B	64	LEU
1	B	66	GLY
1	B	124	GLU
1	B	160	GLY
1	B	237	ASP
1	B	252	ALA
1	B	267	ASP
1	A	92	ASP
1	A	124	GLU
1	A	232	PHE
1	A	300	PHE
1	A	324	ILE
1	B	161	GLY
1	B	164	GLN
1	B	175	SER
1	A	11	LEU
1	A	55	ALA
1	A	117	GLN
1	B	54	PRO
1	B	214	ALA
1	A	54	PRO
1	A	346	VAL
1	A	168	GLY
1	A	321	GLY

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	256/283 (90%)	212 (83%)	44 (17%)	2	6
1	B	180/283 (64%)	147 (82%)	33 (18%)	1	5
All	All	436/566 (77%)	359 (82%)	77 (18%)	2	5

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	26	LEU
1	A	39	THR
1	A	57	LEU
1	A	58	VAL
1	A	72	ASN
1	A	73	LYS
1	A	95	GLN
1	A	97	ASN
1	A	98	SER
1	A	102	LYS
1	A	104	ARG
1	A	119	GLU
1	A	120	LEU
1	A	133	GLN
1	A	140	GLN
1	A	151	ARG
1	A	169	HIS
1	A	184	LEU
1	A	193	ASN
1	A	199	LEU
1	A	222	VAL
1	A	227	SER
1	A	243	VAL
1	A	244	ARG
1	A	246	VAL
1	A	249	ILE
1	A	260	ARG
1	A	269	ARG
1	A	270	LEU
1	A	279	THR
1	A	288	ILE
1	A	295	ILE
1	A	296	VAL

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Mol	Chain	Res	Type
1	A	300	PHE
1	A	301	TYR
1	A	302	THR
1	A	303	ARG
1	A	316	ARG
1	A	318	ILE
1	A	319	LYS
1	A	328	MET
1	A	342	VAL
1	A	348	LEU
1	B	50	ILE
1	B	51	GLU
1	B	57	LEU
1	B	60	VAL
1	B	71	LEU
1	B	72	ASN
1	B	75	LEU
1	B	79	VAL
1	B	92	ASP
1	B	95	GLN
1	B	112	ARG
1	B	120	LEU
1	B	128	LYS
1	B	132	GLU
1	B	133	GLN
1	B	135	GLN
1	B	155	LEU
1	B	162	THR
1	B	163	LEU
1	B	178	ASN
1	B	183	ASP
1	B	184	LEU
1	B	188	THR
1	B	217	LYS
1	B	224	VAL
1	B	231	LYS
1	B	232	PHE
1	B	244	ARG
1	B	260	ARG
1	B	261	MET
1	B	267	ASP
1	B	281	LEU

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Mol	Chain	Res	Type
1	B	282	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	GLN
1	B	221	HIS
1	B	226	GLN
1	B	265	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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	341/359 (94%)	0.24	11 (3%)	47	37	53, 79, 139, 218	0
1	B	245/359 (68%)	0.32	14 (5%)	23	15	59, 86, 144, 268	0
All	All	586/718 (81%)	0.27	25 (4%)	35	25	53, 83, 144, 268	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	ILE	12.4
1	B	167	GLY	9.2
1	A	127	ALA	8.2
1	B	166	GLY	6.4
1	A	125	ILE	6.0
1	B	124	GLU	5.8
1	B	123	SER	5.5
1	A	123	SER	5.1
1	A	124	GLU	4.6
1	B	165	ALA	4.5
1	A	167	GLY	3.6
1	B	40	VAL	3.4
1	B	163	LEU	2.7
1	B	126	ALA	2.6
1	B	41	ALA	2.5
1	B	235	TYR	2.4
1	A	128	LYS	2.3
1	A	71	LEU	2.3
1	A	13	HIS	2.3
1	A	171	LEU	2.3
1	B	129	ARG	2.2
1	A	168	GLY	2.1
1	B	168	GLY	2.1
1	A	170	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	281	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 ⓘ

There are no carbohydrates 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	360	1/1	0.99	0.17	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.