Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 06:31 PM EST

PDB ID	:	3KJX
Title	:	Crystal structure of a transcriptional regulator, Lacl family protein from Silicibacter pomeroyi
Authors	:	Palani, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-11-03
Resolution	:	2.33 Å(reported)

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

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

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

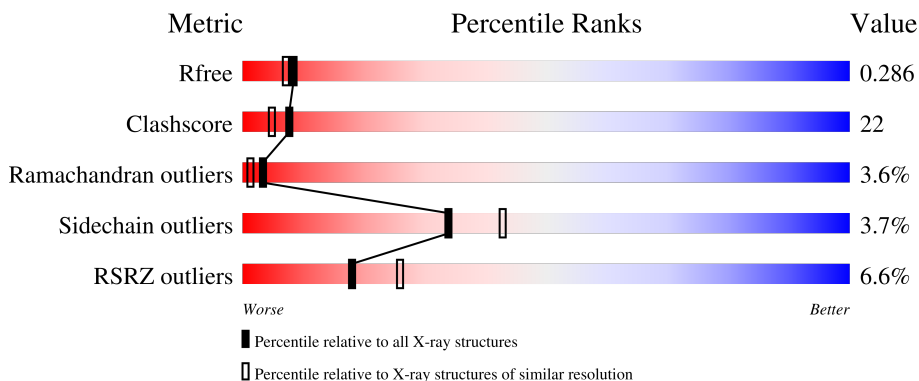|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.33 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		0.286
Clashscore		22
Ramachandran outliers		3.6%
Sidechain outliers		3.7%
RSRZ outliers		6.6%

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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	344	10% / 62% / 30% / 5% · ·
1	B	344	4% / 65% / 28% · ·
1	C	344	6% / 55% / 38% · ·
1	D	344	6% / 61% / 33% · · ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10352 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 Transcriptional regulator, LacI family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	Se	0	0	0
			2552	1603	448	487	1	13			
1	B	333	Total	C	N	O	S	Se	0	0	0
			2552	1603	448	487	1	13			
1	C	333	Total	C	N	O	S	Se	0	0	0
			2552	1603	448	487	1	13			
1	D	335	Total	C	N	O	S	Se	0	0	0
			2572	1615	454	489	1	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q5LM80
A	0	SER	-	expression tag	UNP Q5LM80
A	1	LEU	-	expression tag	UNP Q5LM80
A	341	GLU	-	expression tag	UNP Q5LM80
A	342	GLY	-	expression tag	UNP Q5LM80
B	-1	MSE	-	expression tag	UNP Q5LM80
B	0	SER	-	expression tag	UNP Q5LM80
B	1	LEU	-	expression tag	UNP Q5LM80
B	341	GLU	-	expression tag	UNP Q5LM80
B	342	GLY	-	expression tag	UNP Q5LM80
C	-1	MSE	-	expression tag	UNP Q5LM80
C	0	SER	-	expression tag	UNP Q5LM80
C	1	LEU	-	expression tag	UNP Q5LM80
C	341	GLU	-	expression tag	UNP Q5LM80
C	342	GLY	-	expression tag	UNP Q5LM80
D	-1	MSE	-	expression tag	UNP Q5LM80
D	0	SER	-	expression tag	UNP Q5LM80
D	1	LEU	-	expression tag	UNP Q5LM80
D	341	GLU	-	expression tag	UNP Q5LM80
D	342	GLY	-	expression tag	UNP Q5LM80

• Molecule 2 is water.

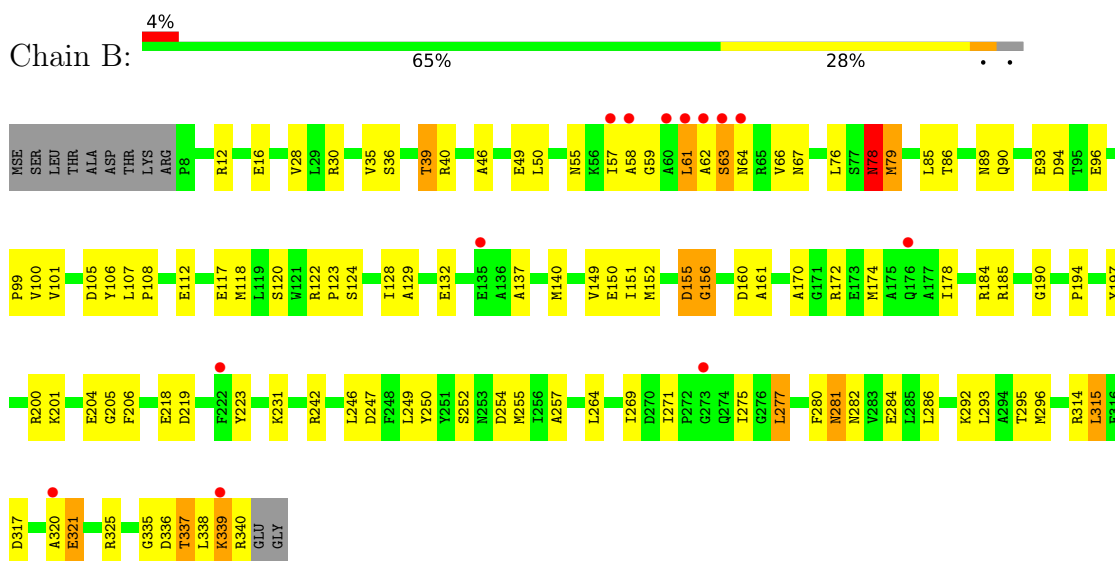| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	36	Total O 36 36	0	0
2	B	25	Total O 25 25	0	0
2	C	30	Total O 30 30	0	0
2	D	33	Total O 33 33	0	0

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.

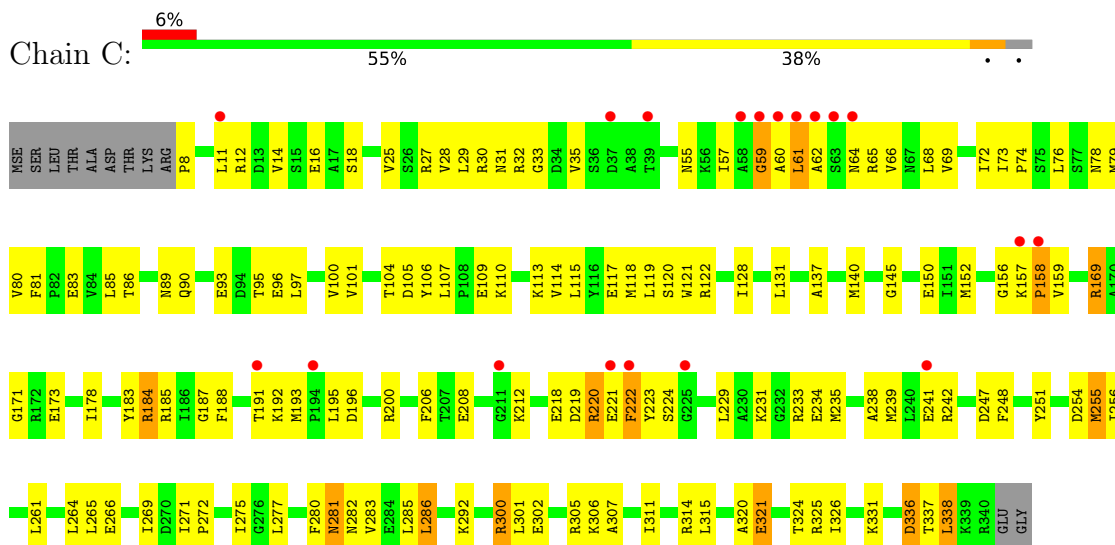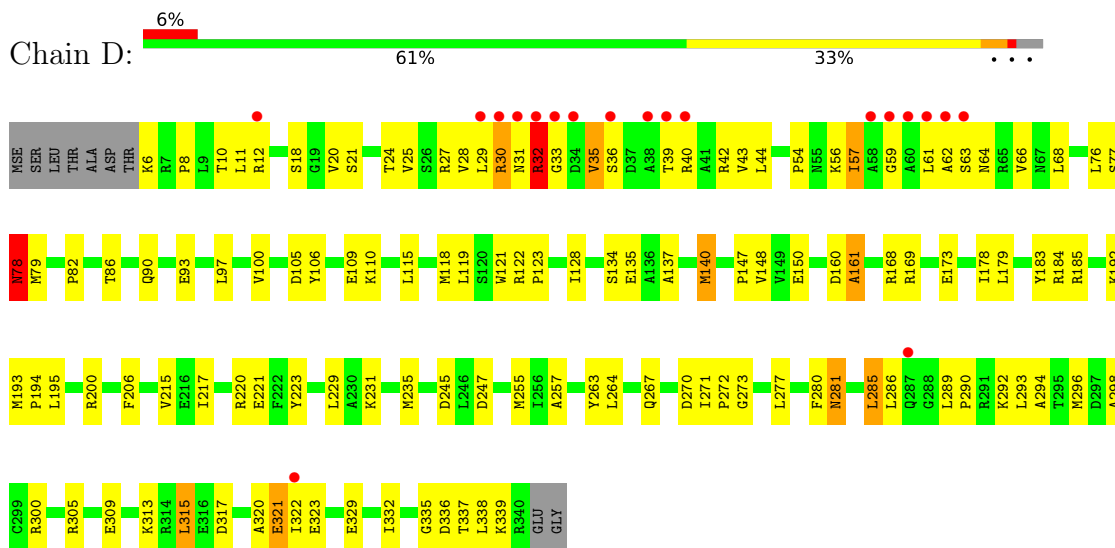• Molecule 1: Transcriptional regulator, LacI family

Chain A:

• Molecule 1: Transcriptional regulator, LacI family

Chain B:

• Molecule 1: Transcriptional regulator, LacI family

Chain C:

• Molecule 1: Transcriptional regulator, LacI family

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.66Å 137.39Å 154.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.29 – 2.33 41.29 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.7 (41.29-2.33) 92.7 (41.29-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.287 0.238 , 0.286	Depositor DCC
R_{free} test set	3076 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.1	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10352	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.38	1/2574 (0.0%)	0.64	0/3451
1	B	0.33	0/2574	0.61	0/3451
1	C	0.37	0/2574	0.63	1/3451 (0.0%)
1	D	0.37	0/2594	0.65	0/3477
All	All	0.36	1/10316 (0.0%)	0.63	1/13830 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	VAL	CA-CB	-5.44	1.43	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	ARG	N-CA-C	-5.48	96.21	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2552	0	2609	118	0
1	B	2552	0	2609	99	0
1	C	2552	0	2609	136	0
1	D	2572	0	2634	133	0

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W O R L D W I D E
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	0	2	0
2	B	25	0	0	1	0
2	C	30	0	0	1	0
2	D	33	0	0	3	0
All	All	10352	0	10461	452	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 22.

All (452) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:LEU:HG	1:C:269:ILE:HD11	1.24	1.18
1:C:115:LEU:HD23	1:C:140:MSE:HE3	1.40	1.03
1:C:137:ALA:HA	1:C:140:MSE:HE2	1.43	1.00
1:B:249:LEU:HG	1:B:275:ILE:HD11	1.44	0.99
1:B:137:ALA:HA	1:B:140:MSE:HE3	1.45	0.99
1:D:28:VAL:HG21	1:D:43:VAL:HG21	1.45	0.97
1:C:95:THR:HG22	1:C:97:LEU:H	1.27	0.94
1:D:137:ALA:HA	1:D:140:MSE:HE2	1.47	0.94
1:B:277:LEU:HD12	1:B:337:THR:HB	1.52	0.92
1:C:283:VAL:HA	1:C:300:ARG:HH12	1.36	0.90
1:D:20:VAL:HG21	1:D:43:VAL:HG22	1.53	0.89
1:D:294:ALA:H	1:D:337:THR:CG2	1.86	0.88
1:A:255:MSE:HE2	1:A:255:MSE:HA	1.52	0.88
1:D:61:LEU:HA	1:D:122:ARG:HE	1.39	0.86
1:D:322:ILE:HG22	1:D:323:GLU:H	1.39	0.86
1:A:55:ASN:HD22	1:B:61:LEU:H	1.23	0.84
1:A:100:VAL:HB	1:B:100:VAL:HG13	1.60	0.83
1:C:60:ALA:N	1:C:64:ASN:HB2	1.94	0.83
1:C:114:VAL:HG12	1:C:118:MSE:HE2	1.59	0.83
1:D:115:LEU:HD23	1:D:140:MSE:HE3	1.62	0.81
1:A:31:ASN:HA	1:A:40:ARG:HH22	1.44	0.81
1:B:271:ILE:HG22	1:B:337:THR:HA	1.62	0.81
1:B:59:GLY:HA3	1:B:64:ASN:HB3	1.63	0.81
1:D:289:LEU:HB3	1:D:290:PRO:HD2	1.60	0.81
1:D:294:ALA:H	1:D:337:THR:HG21	1.45	0.81
1:C:72:ILE:HG12	1:C:118:MSE:HE1	1.63	0.81
1:A:89:ASN:O	1:A:93:GLU:HG2	1.82	0.79
1:B:280:PHE:HE1	1:B:296:MSE:HE2	1.47	0.78
1:D:195:LEU:HD23	2:D:348:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:CG1	1:C:118:MSE:HE2	2.14	0.78
1:D:338:LEU:HD23	1:D:339:LYS:N	1.99	0.78
1:C:137:ALA:HA	1:C:140:MSE:CE	2.15	0.77
1:B:30:ARG:HH22	1:B:58:ALA:HB2	1.48	0.77
1:D:322:ILE:HG22	1:D:323:GLU:N	1.99	0.77
1:C:120:SER:HB2	1:D:56:LYS:HG2	1.67	0.77
2:A:376:HOH:O	1:D:221:GLU:HG3	1.86	0.75
1:D:40:ARG:NH1	1:D:44:LEU:HD11	2.02	0.74
1:A:255:MSE:CE	1:A:255:MSE:HA	2.17	0.74
1:A:100:VAL:HB	1:B:100:VAL:CG1	2.17	0.74
1:A:15:SER:O	1:A:19:GLY:N	2.21	0.74
1:D:32:ARG:HD3	1:D:32:ARG:N	2.04	0.73
1:B:78:ASN:O	1:B:79:MSE:HG2	1.90	0.72
1:A:55:ASN:ND2	1:B:61:LEU:H	1.87	0.71
1:C:208:GLU:O	1:C:212:LYS:HG2	1.90	0.71
1:A:35:VAL:HG13	1:A:39:THR:HB	1.73	0.71
1:B:89:ASN:O	1:B:93:GLU:HG2	1.91	0.71
1:C:62:ALA:HA	1:C:65:ARG:HH11	1.54	0.71
1:A:35:VAL:CG1	1:A:39:THR:HB	2.21	0.70
1:C:145:GLY:HA3	1:D:8:PRO:HB3	1.71	0.70
1:D:33:GLY:O	1:D:35:VAL:HG23	1.91	0.70
1:C:100:VAL:HB	1:D:100:VAL:HG22	1.72	0.70
1:A:200:ARG:O	1:A:204:GLU:HG3	1.90	0.70
1:C:79:MSE:HE1	2:D:364:HOH:O	1.91	0.70
1:A:27:ARG:NH1	1:A:33:GLY:HA3	2.06	0.70
1:D:61:LEU:HA	1:D:122:ARG:NE	2.07	0.69
1:A:255:MSE:HE1	1:A:285:LEU:HD13	1.73	0.69
1:D:286:LEU:HD11	1:D:293:LEU:HD23	1.74	0.69
1:D:293:LEU:HD12	1:D:337:THR:HG21	1.74	0.69
1:C:95:THR:HG22	1:C:97:LEU:N	2.05	0.68
1:D:10:THR:O	1:D:12:ARG:N	2.27	0.68
1:A:186:ILE:HG22	1:A:187:GLY:N	2.08	0.68
1:B:185:ARG:HB3	1:B:218:GLU:OE1	1.94	0.68
1:D:24:THR:O	1:D:28:VAL:HG23	1.93	0.68
1:A:27:ARG:HD3	1:A:32:ARG:HD3	1.75	0.67
1:D:29:LEU:O	1:D:30:ARG:HG2	1.94	0.67
1:C:57:ILE:HD13	1:D:121:TRP:O	1.95	0.67
1:D:21:SER:O	1:D:25:VAL:HG23	1.94	0.67
1:C:277:LEU:HB3	2:C:346:HOH:O	1.93	0.67
1:D:115:LEU:HD23	1:D:140:MSE:CE	2.24	0.67
1:B:170:ALA:HB2	1:B:296:MSE:HE1	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:367:HOH:O	1:B:96:GLU:HG3	1.95	0.67
1:D:338:LEU:HD23	1:D:339:LYS:H	1.57	0.67
1:D:221:GLU:HB3	1:D:235:MSE:HE2	1.77	0.66
1:C:95:THR:HG22	1:C:96:GLU:N	2.11	0.66
1:D:57:ILE:HG22	1:D:66:VAL:HG11	1.78	0.66
1:C:57:ILE:HG23	1:D:121:TRP:HA	1.78	0.66
1:D:338:LEU:O	1:D:339:LYS:HB2	1.93	0.66
1:A:18:SER:OG	1:A:43:VAL:HG12	1.96	0.66
1:C:72:ILE:HG12	1:C:118:MSE:CE	2.26	0.66
1:D:322:ILE:CG2	1:D:323:GLU:H	2.09	0.65
1:C:219:ASP:OD2	1:C:239:MSE:HG3	1.97	0.65
1:A:185:ARG:HB3	1:A:218:GLU:OE1	1.96	0.64
1:D:59:GLY:HA2	1:D:64:ASN:HB3	1.78	0.64
1:C:238:ALA:O	1:C:241:GLU:HB3	1.98	0.64
1:B:35:VAL:HG12	1:B:39:THR:HG23	1.80	0.64
1:D:270:ASP:OD2	1:D:273:GLY:HA3	1.98	0.64
1:B:277:LEU:CD1	1:B:337:THR:HB	2.27	0.63
1:B:264:LEU:HG	1:B:269:ILE:HD11	1.78	0.63
1:A:187:GLY:HA2	1:A:219:ASP:O	1.98	0.63
1:C:191:THR:HG22	1:C:223:TYR:HB3	1.81	0.63
1:A:11:LEU:C	1:A:13:ASP:H	2.02	0.63
1:A:55:ASN:HD22	1:B:61:LEU:N	1.95	0.63
1:B:280:PHE:O	1:B:281:ASN:HB2	1.98	0.62
1:B:190:GLY:HA2	1:B:252:SER:HB2	1.79	0.62
1:C:76:LEU:HD13	1:D:76:LEU:HD22	1.81	0.62
1:B:46:ALA:O	1:B:49:GLU:HG2	1.98	0.62
1:A:92:LEU:HD12	1:A:99:PRO:HG3	1.81	0.62
1:D:271:ILE:HD12	1:D:277:LEU:HD11	1.82	0.62
1:C:280:PHE:O	1:C:281:ASN:HB2	1.98	0.62
1:C:157:LYS:NZ	1:C:157:LYS:HB2	2.15	0.61
1:B:36:SER:OG	1:B:39:THR:HG22	2.00	0.61
1:B:320:ALA:O	1:B:321:GLU:HB3	2.00	0.61
1:B:339:LYS:O	1:B:340:ARG:HB3	1.99	0.61
1:C:115:LEU:CD2	1:C:140:MSE:HE3	2.26	0.61
1:D:115:LEU:CD2	1:D:140:MSE:HE3	2.31	0.61
1:C:192:LYS:HG3	1:C:196:ASP:HB2	1.83	0.61
1:A:57:ILE:HD11	1:B:57:ILE:HG21	1.83	0.60
1:A:21:SER:O	1:A:22:GLU:HB2	2.00	0.60
1:C:121:TRP:HA	1:D:57:ILE:HG23	1.83	0.60
1:C:89:ASN:O	1:C:93:GLU:HG2	2.02	0.60
1:A:39:THR:HA	1:A:42:ARG:NE	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:O	1:A:90:GLN:HG3	2.02	0.60
1:A:39:THR:O	1:A:42:ARG:HB3	2.02	0.60
1:B:132:GLU:HG2	1:B:197:TYR:CD2	2.37	0.60
1:B:112:GLU:HG3	1:B:140:MSE:CE	2.31	0.60
1:A:12:ARG:HG3	1:A:12:ARG:O	2.01	0.60
1:C:105:ASP:O	1:C:106:TYR:HB2	2.02	0.60
1:B:155:ASP:OD1	1:B:201:LYS:HD3	2.02	0.59
1:B:12:ARG:O	1:B:16:GLU:HG3	2.02	0.59
1:B:280:PHE:CE1	1:B:296:MSE:HE2	2.35	0.59
1:C:283:VAL:HA	1:C:300:ARG:NH1	2.11	0.59
1:A:322:ILE:HG13	1:A:323:GLU:H	1.67	0.59
1:D:119:LEU:HD12	1:D:140:MSE:HG2	1.84	0.59
1:D:30:ARG:O	1:D:31:ASN:HB2	2.02	0.59
1:C:60:ALA:H	1:C:64:ASN:HB2	1.67	0.59
1:C:221:GLU:O	1:C:221:GLU:HG3	2.01	0.59
1:A:27:ARG:HD2	1:A:33:GLY:H	1.66	0.59
1:C:95:THR:CG2	1:C:96:GLU:N	2.66	0.59
1:A:83:GLU:HB3	1:A:300:ARG:HD2	1.85	0.59
1:B:79:MSE:HG3	1:B:255:MSE:CE	2.33	0.59
1:C:301:LEU:O	1:C:305:ARG:HG3	2.02	0.59
1:C:27:ARG:HE	1:C:32:ARG:HH12	1.51	0.59
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.68	0.58
1:B:184:ARG:O	1:B:247:ASP:OD1	2.22	0.58
1:B:336:ASP:O	1:B:338:LEU:N	2.37	0.58
1:D:20:VAL:HG12	1:D:42:ARG:HH21	1.68	0.58
1:A:40:ARG:O	1:A:44:LEU:HG	2.03	0.58
1:A:38:ALA:O	1:A:42:ARG:HB2	2.03	0.58
1:A:92:LEU:CD1	1:A:99:PRO:HG3	2.33	0.58
1:D:27:ARG:HG3	1:D:32:ARG:HH21	1.68	0.58
1:A:280:PHE:O	1:A:281:ASN:HB2	2.03	0.58
1:C:93:GLU:OE2	1:D:110:LYS:HE3	2.04	0.58
1:D:86:THR:O	1:D:90:GLN:HG3	2.04	0.58
1:B:59:GLY:CA	1:B:64:ASN:HB3	2.32	0.58
1:A:83:GLU:HA	1:A:83:GLU:OE1	2.03	0.57
1:B:174:MSE:HG2	1:B:250:TYR:CE1	2.40	0.57
1:D:28:VAL:HG11	1:D:43:VAL:HB	1.86	0.57
1:D:305:ARG:O	1:D:309:GLU:HG3	2.04	0.57
1:D:294:ALA:N	1:D:337:THR:CG2	2.64	0.57
1:B:105:ASP:O	1:B:106:TYR:HB2	2.03	0.57
1:D:39:THR:O	1:D:43:VAL:HG23	2.05	0.57
1:A:68:LEU:HD22	1:A:123:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:O	1:A:26:SER:N	2.38	0.56
1:B:124:SER:HB3	1:B:315:LEU:HD21	1.86	0.56
1:C:80:VAL:HA	1:C:300:ARG:HD2	1.87	0.56
1:A:186:ILE:O	1:A:248:PHE:O	2.22	0.56
1:B:86:THR:O	1:B:90:GLN:HG3	2.05	0.56
1:C:233:ARG:NH2	1:C:266:GLU:OE1	2.38	0.56
1:C:100:VAL:HB	1:D:100:VAL:CG2	2.36	0.56
1:A:56:LYS:HB2	1:B:120:SER:HB2	1.88	0.56
1:C:187:GLY:HA2	1:C:219:ASP:O	2.06	0.56
1:D:280:PHE:O	1:D:281:ASN:HB2	2.05	0.56
1:D:20:VAL:HG23	1:D:25:VAL:HG22	1.89	0.56
1:A:122:ARG:HH21	1:B:55:ASN:HB2	1.71	0.55
1:B:320:ALA:O	1:B:321:GLU:CB	2.53	0.55
1:D:134:SER:O	1:D:135:GLU:HB3	2.06	0.55
1:D:57:ILE:O	1:D:57:ILE:HG13	2.05	0.55
1:A:186:ILE:HD12	1:A:186:ILE:N	2.22	0.55
1:C:57:ILE:CG2	1:D:121:TRP:HA	2.36	0.55
1:C:114:VAL:HG12	1:C:118:MSE:CE	2.34	0.55
1:D:30:ARG:HA	1:D:30:ARG:HE	1.72	0.55
1:A:27:ARG:CD	1:A:32:ARG:HB3	2.37	0.55
1:C:193:MSE:HE2	1:C:222:PHE:CE2	2.41	0.55
1:A:221:GLU:HG3	1:A:235:MSE:HE3	1.87	0.54
1:A:162:MSE:HE2	1:A:325:ARG:HB3	1.88	0.54
1:C:193:MSE:HE3	1:C:200:ARG:HG2	1.89	0.54
1:B:264:LEU:CG	1:B:269:ILE:HD11	2.37	0.54
1:D:313:LYS:HE3	1:D:322:ILE:HG13	1.89	0.54
1:A:76:LEU:HD13	1:B:76:LEU:HD22	1.88	0.54
1:C:61:LEU:HG	1:C:122:ARG:HH21	1.72	0.54
1:A:40:ARG:C	1:A:42:ARG:H	2.10	0.54
1:B:172:ARG:HG2	1:B:205:GLY:O	2.08	0.54
1:D:79:MSE:HE2	1:D:255:MSE:HE3	1.89	0.54
1:A:27:ARG:HD3	1:A:32:ARG:HB3	1.90	0.54
1:B:57:ILE:O	1:B:57:ILE:HG13	2.08	0.54
1:A:322:ILE:HG13	1:A:323:GLU:N	2.23	0.53
1:C:285:LEU:HD11	1:D:285:LEU:HD11	1.90	0.53
1:B:79:MSE:HG3	1:B:255:MSE:HE1	1.91	0.53
1:C:223:TYR:CE2	1:C:231:LYS:HE2	2.43	0.53
1:B:89:ASN:ND2	1:B:99:PRO:HG3	2.24	0.53
1:A:18:SER:O	1:A:20:VAL:HG23	2.09	0.53
1:B:264:LEU:HG	1:B:269:ILE:CD1	2.39	0.53
1:D:148:VAL:O	1:D:161:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:NH2	1:B:58:ALA:HB2	2.22	0.52
1:A:147:PRO:HB3	1:A:314:ARG:NH1	2.25	0.52
1:B:170:ALA:CB	1:B:296:MSE:HE1	2.39	0.52
1:B:325:ARG:HD2	2:B:366:HOH:O	2.08	0.52
1:C:14:VAL:O	1:C:18:SER:HB2	2.09	0.52
1:A:237:GLN:HG3	1:A:238:ALA:N	2.24	0.52
1:A:67:ASN:ND2	1:B:117:GLU:OE1	2.42	0.52
1:A:204:GLU:O	1:A:208:GLU:HG3	2.09	0.52
1:A:9:LEU:C	1:A:9:LEU:HD23	2.29	0.52
1:B:194:PRO:HA	1:B:200:ARG:HD2	1.91	0.52
1:C:184:ARG:O	1:C:247:ASP:OD1	2.28	0.52
1:D:28:VAL:HG13	1:D:40:ARG:HG3	1.92	0.52
1:A:27:ARG:CZ	1:A:33:GLY:HA3	2.38	0.52
1:B:174:MSE:O	1:B:178:ILE:HG13	2.10	0.52
1:C:169:ARG:NH1	1:C:169:ARG:HG3	2.24	0.52
1:A:52:TYR:OH	1:B:61:LEU:HD21	2.09	0.52
1:C:81:PHE:O	1:C:85:LEU:HG	2.10	0.52
1:D:18:SER:OG	1:D:20:VAL:HG22	2.10	0.52
1:D:30:ARG:HB3	1:D:32:ARG:HD2	1.91	0.52
1:A:255:MSE:HE1	1:A:285:LEU:HD22	1.92	0.51
1:C:86:THR:O	1:C:90:GLN:HG3	2.10	0.51
1:D:178:ILE:CG2	1:D:183:TYR:HB2	2.40	0.51
1:B:112:GLU:HG3	1:B:140:MSE:HE1	1.91	0.51
1:C:72:ILE:HD11	1:C:118:MSE:HE3	1.92	0.51
1:D:79:MSE:HE2	1:D:255:MSE:SE	2.61	0.51
1:B:178:ILE:HD12	1:B:206:PHE:HE1	1.76	0.51
1:C:220:ARG:HG2	1:C:220:ARG:HH11	1.76	0.51
1:A:79:MSE:HE1	1:A:285:LEU:HD13	1.91	0.51
1:C:72:ILE:CG1	1:C:118:MSE:HE1	2.39	0.51
1:C:183:TYR:OH	1:C:272:PRO:HB2	2.11	0.51
1:B:190:GLY:HA2	1:B:252:SER:CB	2.40	0.50
1:B:249:LEU:CG	1:B:275:ILE:HD11	2.29	0.50
1:D:160:ASP:O	1:D:161:ALA:O	2.30	0.50
1:B:219:ASP:OD2	1:B:242:ARG:HD2	2.12	0.50
1:C:306:LYS:HE3	1:C:326:ILE:CD1	2.42	0.50
1:D:115:LEU:CG	1:D:140:MSE:HE3	2.42	0.50
1:C:8:PRO:HB2	1:D:62:ALA:HB2	1.94	0.50
1:C:255:MSE:SE	1:C:285:LEU:HD13	2.61	0.50
1:A:198:ARG:HH11	1:A:198:ARG:HG3	1.77	0.50
1:A:36:SER:O	1:A:40:ARG:HG2	2.12	0.50
1:C:27:ARG:HE	1:C:32:ARG:NH1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLU:HG3	1:B:50:LEU:N	2.27	0.49
1:C:83:GLU:HG2	1:C:300:ARG:HE	1.77	0.49
1:B:317:ASP:HB3	1:B:320:ALA:HB2	1.94	0.49
1:D:148:VAL:O	1:D:160:ASP:O	2.29	0.49
1:D:193:MSE:HE3	1:D:200:ARG:HA	1.95	0.49
1:A:280:PHE:O	1:A:281:ASN:CB	2.60	0.49
1:C:220:ARG:HD2	1:C:220:ARG:O	2.12	0.49
1:D:6:LYS:HB3	1:D:6:LYS:NZ	2.26	0.49
1:C:192:LYS:HD3	1:C:192:LYS:O	2.13	0.49
1:C:193:MSE:HA	1:C:195:LEU:H	1.77	0.49
1:D:292:LYS:O	1:D:335:GLY:HA3	2.13	0.49
1:C:95:THR:CG2	1:C:96:GLU:H	2.26	0.49
1:B:277:LEU:HD13	1:B:293:LEU:CD1	2.42	0.49
1:C:277:LEU:HD23	1:C:277:LEU:N	2.28	0.49
1:C:85:LEU:HD13	1:C:101:VAL:HG21	1.95	0.48
1:D:105:ASP:O	1:D:106:TYR:HB2	2.13	0.48
1:D:280:PHE:O	1:D:281:ASN:CB	2.60	0.48
1:A:68:LEU:HD23	1:A:68:LEU:C	2.34	0.48
1:D:257:ALA:HB1	1:D:293:LEU:HD21	1.96	0.48
1:A:11:LEU:C	1:A:13:ASP:N	2.66	0.48
1:A:128:ILE:O	1:A:150:GLU:HA	2.13	0.48
1:A:85:LEU:HD22	1:A:101:VAL:HG21	1.95	0.48
1:C:169:ARG:HH11	1:C:169:ARG:HG3	1.78	0.48
1:B:155:ASP:O	1:B:156:GLY:O	2.32	0.48
1:C:221:GLU:HB3	1:C:242:ARG:HH22	1.77	0.48
1:C:229:LEU:HD12	1:C:255:MSE:HG3	1.96	0.48
1:C:251:TYR:HB3	1:C:256:ILE:HG13	1.96	0.48
1:C:261:LEU:O	1:C:265:LEU:HG	2.14	0.48
1:D:296:MSE:HE3	1:D:332:ILE:HG13	1.94	0.48
1:A:93:GLU:O	1:A:95:THR:N	2.46	0.47
1:D:221:GLU:HB3	1:D:235:MSE:CE	2.44	0.47
1:D:20:VAL:HG23	1:D:25:VAL:CG2	2.44	0.47
1:C:191:THR:HA	1:C:223:TYR:O	2.14	0.47
1:B:218:GLU:HB3	1:B:246:LEU:HD21	1.96	0.47
1:C:11:LEU:HD22	1:C:25:VAL:HG12	1.96	0.47
1:A:255:MSE:HE1	1:A:285:LEU:CD1	2.44	0.47
1:D:322:ILE:CG2	1:D:323:GLU:N	2.68	0.47
1:A:121:TRP:CD1	1:B:66:VAL:HG21	2.50	0.47
1:C:83:GLU:HB3	1:C:300:ARG:HG2	1.96	0.47
1:A:174:MSE:HG2	1:A:250:TYR:CE1	2.49	0.47
1:B:62:ALA:O	1:B:63:SER:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:TYR:CD2	1:C:231:LYS:HE2	2.50	0.47
1:D:229:LEU:HD12	1:D:255:MSE:HG3	1.97	0.47
1:A:105:ASP:O	1:A:106:TYR:HB2	2.14	0.46
1:C:221:GLU:OE2	1:C:235:MSE:HG2	2.15	0.46
1:C:78:ASN:O	1:C:79:MSE:HE2	2.15	0.46
1:C:193:MSE:HA	1:C:195:LEU:N	2.31	0.46
1:C:307:ALA:O	1:C:311:ILE:HG12	2.14	0.46
1:A:311:ILE:O	1:A:315:LEU:HD13	2.15	0.46
1:C:272:PRO:HA	1:C:275:ILE:O	2.15	0.46
1:D:82:PRO:HG2	2:D:364:HOH:O	2.16	0.46
1:B:254:ASP:OD2	1:B:282:ASN:N	2.48	0.46
1:D:118:MSE:O	1:D:123:PRO:HD3	2.15	0.46
1:A:27:ARG:HD2	1:A:33:GLY:N	2.31	0.46
1:B:149:VAL:HG22	1:B:161:ALA:HB3	1.98	0.46
1:C:314:ARG:NH2	1:C:324:THR:HG21	2.31	0.46
1:B:61:LEU:HG	1:B:122:ARG:HH21	1.80	0.46
1:C:113:LYS:O	1:C:117:GLU:HG2	2.16	0.46
1:C:32:ARG:HG2	1:C:33:GLY:N	2.30	0.46
1:D:115:LEU:HB3	1:D:140:MSE:HE3	1.98	0.46
1:D:179:LEU:HD21	1:D:215:VAL:HG11	1.97	0.46
1:A:198:ARG:HG3	1:A:198:ARG:NH1	2.31	0.46
1:C:271:ILE:CG2	1:C:337:THR:HG22	2.46	0.46
1:A:192:LYS:HB2	1:A:192:LYS:NZ	2.31	0.46
1:A:276:GLY:C	1:A:277:LEU:HD12	2.36	0.46
1:D:317:ASP:OD2	1:D:320:ALA:HB2	2.15	0.46
1:D:40:ARG:HH12	1:D:44:LEU:HD11	1.77	0.46
1:D:77:SER:C	1:D:78:ASN:O	2.52	0.46
1:A:149:VAL:HG22	1:A:161:ALA:HB3	1.98	0.46
1:B:61:LEU:HB3	1:B:62:ALA:H	1.50	0.46
1:D:20:VAL:HG21	1:D:43:VAL:CG2	2.37	0.46
1:D:272:PRO:HB3	1:D:337:THR:O	2.16	0.46
1:C:231:LYS:HG3	1:C:235:MSE:HE3	1.97	0.46
1:A:83:GLU:HB2	1:A:300:ARG:NH1	2.31	0.45
1:C:55:ASN:ND2	1:D:61:LEU:H	2.14	0.45
1:C:157:LYS:HB3	1:C:325:ARG:NH1	2.31	0.45
1:D:298:ALA:HB3	1:D:300:ARG:HG3	1.98	0.45
1:A:189:MSE:HG2	1:A:221:GLU:HB3	1.98	0.45
1:D:79:MSE:O	1:D:300:ARG:NH1	2.49	0.45
1:C:121:TRP:CZ3	1:D:68:LEU:HD12	2.52	0.45
1:C:109:GLU:CD	1:C:109:GLU:H	2.20	0.45
1:C:280:PHE:O	1:C:281:ASN:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PHE:O	1:B:281:ASN:CB	2.64	0.45
1:B:85:LEU:HD22	1:B:101:VAL:HG21	1.99	0.45
1:C:72:ILE:CG1	1:C:118:MSE:CE	2.95	0.45
1:C:80:VAL:O	1:C:300:ARG:HG2	2.17	0.45
1:C:188:PHE:HB3	1:C:220:ARG:HB3	2.00	0.44
1:A:184:ARG:O	1:A:247:ASP:OD1	2.35	0.44
1:A:317:ASP:O	1:A:320:ALA:N	2.47	0.44
1:A:319:GLU:O	1:A:320:ALA:C	2.56	0.44
1:C:157:LYS:HB2	1:C:157:LYS:HZ3	1.82	0.44
1:D:293:LEU:HA	1:D:337:THR:HG21	1.99	0.44
1:A:29:LEU:HD12	1:A:44:LEU:CD2	2.47	0.44
1:D:169:ARG:O	1:D:173:GLU:HB2	2.18	0.44
1:D:285:LEU:C	1:D:285:LEU:HD23	2.38	0.44
1:C:30:ARG:O	1:C:31:ASN:HB2	2.16	0.44
1:D:264:LEU:HD23	1:D:271:ILE:HD11	1.98	0.44
1:D:29:LEU:HD22	1:D:54:PRO:HB3	2.00	0.44
1:B:129:ALA:HA	1:B:151:ILE:HG13	1.99	0.44
1:C:320:ALA:O	1:C:321:GLU:HB3	2.18	0.43
1:C:185:ARG:HB3	1:C:218:GLU:OE1	2.17	0.43
1:A:69:VAL:HG23	1:A:97:LEU:HB3	1.99	0.43
1:A:31:ASN:HA	1:A:40:ARG:NH2	2.24	0.43
1:C:28:VAL:C	1:C:30:ARG:H	2.21	0.43
1:D:231:LYS:HA	1:D:231:LYS:HD2	1.86	0.43
1:D:272:PRO:HD3	1:D:336:ASP:O	2.18	0.43
1:B:61:LEU:HA	1:B:122:ARG:HE	1.82	0.43
1:B:315:LEU:HD12	1:B:315:LEU:HA	1.82	0.43
1:B:338:LEU:C	1:B:338:LEU:HD23	2.38	0.43
1:D:97:LEU:HD11	1:D:315:LEU:HD23	2.00	0.43
1:C:229:LEU:HD11	1:C:255:MSE:SE	2.69	0.43
1:D:134:SER:O	1:D:135:GLU:CB	2.67	0.43
1:D:184:ARG:O	1:D:247:ASP:OD1	2.36	0.43
1:A:20:VAL:CG1	1:A:24:THR:OG1	2.67	0.43
1:C:59:GLY:HA3	1:C:64:ASN:HB3	2.00	0.43
1:A:24:THR:O	1:A:25:VAL:C	2.57	0.43
1:A:27:ARG:HD3	1:A:32:ARG:CD	2.44	0.43
1:A:83:GLU:HB2	1:A:300:ARG:HH11	1.84	0.43
1:B:292:LYS:O	1:B:335:GLY:O	2.37	0.43
1:C:183:TYR:CD2	1:C:248:PHE:HB2	2.54	0.43
1:D:192:LYS:HA	1:D:192:LYS:HD3	1.76	0.43
1:B:35:VAL:CG1	1:B:39:THR:HG23	2.47	0.43
1:C:171:GLY:O	1:C:206:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ILE:HG21	1:C:337:THR:HG22	2.01	0.43
1:C:61:LEU:HB3	1:C:62:ALA:H	1.53	0.43
1:D:184:ARG:O	1:D:247:ASP:CG	2.57	0.43
1:A:160:ASP:OD2	1:A:314:ARG:NH2	2.52	0.43
1:B:257:ALA:HB1	1:B:293:LEU:HD21	2.01	0.43
1:B:295:THR:OG1	1:B:296:MSE:N	2.51	0.43
1:A:160:ASP:CG	1:A:314:ARG:HH22	2.21	0.42
1:B:59:GLY:HA3	1:B:64:ASN:HD22	1.84	0.42
1:D:178:ILE:HG22	1:D:183:TYR:HB2	2.01	0.42
1:D:257:ALA:CB	1:D:293:LEU:HD21	2.49	0.42
1:A:118:MSE:O	1:A:123:PRO:HD3	2.19	0.42
1:D:61:LEU:HB3	1:D:62:ALA:H	1.67	0.42
1:A:27:ARG:HD3	1:A:32:ARG:CG	2.49	0.42
1:C:254:ASP:OD2	1:C:282:ASN:N	2.52	0.42
1:D:294:ALA:N	1:D:337:THR:HG22	2.35	0.42
1:A:255:MSE:CE	1:A:285:LEU:HD22	2.49	0.42
1:B:107:LEU:HA	1:B:108:PRO:HD3	1.91	0.42
1:A:122:ARG:NH2	1:B:55:ASN:HB2	2.34	0.42
1:A:326:ILE:N	1:A:326:ILE:HD12	2.34	0.42
1:A:39:THR:HA	1:A:42:ARG:CZ	2.49	0.42
1:B:338:LEU:O	1:B:339:LYS:C	2.58	0.42
1:C:104:THR:O	1:C:110:LYS:HD2	2.20	0.42
1:C:178:ILE:HD12	1:C:206:PHE:HE1	1.85	0.42
1:A:237:GLN:HB2	1:A:263:TYR:CZ	2.54	0.42
1:A:89:ASN:C	1:A:93:GLU:HG2	2.40	0.42
1:C:115:LEU:HD23	1:C:140:MSE:CE	2.29	0.42
1:C:128:ILE:O	1:C:150:GLU:HA	2.20	0.42
1:D:109:GLU:HG2	1:D:110:LYS:N	2.35	0.42
1:D:263:TYR:O	1:D:267:GLN:HG2	2.19	0.42
1:D:206:PHE:CE2	1:D:217:ILE:HD11	2.55	0.42
1:D:293:LEU:HA	1:D:337:THR:CG2	2.49	0.42
1:C:145:GLY:CA	1:D:8:PRO:HB3	2.46	0.42
1:A:65:ARG:HD3	1:A:123:PRO:O	2.20	0.42
1:A:8:PRO:O	1:A:9:LEU:O	2.37	0.42
1:C:12:ARG:O	1:C:16:GLU:HG3	2.20	0.42
1:D:185:ARG:HD3	1:D:245:ASP:O	2.20	0.42
1:A:11:LEU:O	1:A:13:ASP:N	2.52	0.42
1:B:118:MSE:O	1:B:123:PRO:HD3	2.20	0.42
1:C:254:ASP:HB3	1:C:286:LEU:HD11	2.02	0.42
1:D:20:VAL:CG1	1:D:42:ARG:HH21	2.31	0.42
1:C:131:LEU:HD22	1:C:158:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ILE:HB	1:C:74:PRO:HD2	2.01	0.42
1:D:30:ARG:HA	1:D:30:ARG:NE	2.33	0.42
1:A:158:PRO:HB3	1:A:162:MSE:HB2	2.02	0.41
1:A:338:LEU:HD23	1:A:338:LEU:C	2.41	0.41
1:D:147:PRO:HG2	1:D:315:LEU:CD1	2.50	0.41
1:A:124:SER:HB3	1:A:315:LEU:HD21	2.02	0.41
1:A:47:ALA:HB1	1:A:52:TYR:HB3	2.03	0.41
1:A:57:ILE:HD11	1:B:57:ILE:CG2	2.48	0.41
1:B:89:ASN:ND2	1:B:99:PRO:CG	2.83	0.41
1:A:28:VAL:HG11	1:A:40:ARG:HA	2.02	0.41
1:B:184:ARG:O	1:B:185:ARG:CB	2.67	0.41
1:B:94:ASP:OD2	1:C:331:LYS:CB	2.68	0.41
1:A:262:LEU:O	1:A:266:GLU:HB2	2.20	0.41
1:B:128:ILE:O	1:B:150:GLU:HA	2.19	0.41
1:C:285:LEU:HG	1:D:229:LEU:HD22	2.02	0.41
1:D:79:MSE:CE	1:D:255:MSE:HE3	2.49	0.41
1:D:271:ILE:HD12	1:D:277:LEU:CD1	2.49	0.41
1:C:306:LYS:HD2	1:C:306:LYS:HA	1.84	0.41
1:A:55:ASN:ND2	1:B:61:LEU:N	2.60	0.41
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.91	0.41
1:D:289:LEU:HB3	1:D:290:PRO:CD	2.42	0.41
1:D:296:MSE:HE3	1:D:332:ILE:CG1	2.50	0.41
1:C:100:VAL:CG2	1:D:100:VAL:HG21	2.51	0.41
1:A:27:ARG:HD2	1:A:32:ARG:HB3	2.02	0.41
1:B:66:VAL:HG22	1:B:67:ASN:N	2.36	0.41
1:C:233:ARG:HH22	1:C:266:GLU:CD	2.24	0.41
1:C:68:LEU:HD23	1:C:69:VAL:N	2.35	0.41
1:D:79:MSE:HE2	1:D:255:MSE:CE	2.51	0.41
1:A:40:ARG:C	1:A:42:ARG:N	2.74	0.41
1:B:184:ARG:C	1:B:185:ARG:HG3	2.40	0.41
1:B:223:TYR:CE1	1:B:231:LYS:HE2	2.56	0.41
1:C:57:ILE:HD11	1:D:122:ARG:HB2	2.03	0.40
1:C:193:MSE:O	1:C:224:SER:HA	2.21	0.40
1:D:128:ILE:O	1:D:150:GLU:HA	2.22	0.40
1:D:106:TYR:HB3	1:D:195:LEU:HB3	2.01	0.40
1:D:223:TYR:CD2	1:D:231:LYS:HE2	2.56	0.40
1:A:192:LYS:HD3	1:A:192:LYS:HA	1.76	0.40
1:A:167:HIS:O	1:A:202:ARG:HA	2.21	0.40
1:A:264:LEU:HD22	1:A:277:LEU:HD21	2.03	0.40
1:B:28:VAL:HG22	1:B:40:ARG:HG2	2.03	0.40
1:B:160:ASP:CG	1:B:314:ARG:HH12	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HA	1:C:119:LEU:HD23	1.94	0.40
1:C:302:GLU:O	1:C:306:LYS:HB2	2.22	0.40
1:C:57:ILE:HG22	1:C:66:VAL:HG21	2.03	0.40
1:C:283:VAL:O	1:C:286:LEU:HB2	2.21	0.40
1:C:292:LYS:HE2	1:C:336:ASP:OD2	2.22	0.40
1:C:97:LEU:HD11	1:C:315:LEU:HD12	2.04	0.40
1:D:223:TYR:CG	1:D:231:LYS:HE2	2.55	0.40
1:D:320:ALA:O	1:D:321:GLU:O	2.40	0.40
1:A:192:LYS:HB2	1:A:192:LYS:HZ2	1.86	0.40
1:A:83:GLU:CB	1:A:300:ARG:HD2	2.50	0.40
1:C:107:LEU:HD12	1:C:110:LYS:HE3	2.04	0.40
1:C:338:LEU:C	1:C:338:LEU:HD23	2.42	0.40
1:D:27:ARG:HH21	1:D:33:GLY:HA3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	285 (86%)	32 (10%)	14 (4%)	3	1
1	B	331/344 (96%)	303 (92%)	17 (5%)	11 (3%)	4	1
1	C	331/344 (96%)	293 (88%)	26 (8%)	12 (4%)	3	1
1	D	333/344 (97%)	298 (90%)	24 (7%)	11 (3%)	4	1
All	All	1326/1376 (96%)	1179 (89%)	99 (8%)	48 (4%)	3	1

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	22	GLU

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Mol	Chain	Res	Type
1	A	25	VAL
1	A	61	LEU
1	B	61	LEU
1	B	79	MSE
1	B	155	ASP
1	B	156	GLY
1	B	281	ASN
1	B	337	THR
1	C	61	LEU
1	C	158	PRO
1	C	281	ASN
1	D	11	LEU
1	D	161	ALA
1	D	321	GLU
1	A	24	THR
1	A	186	ILE
1	A	281	ASN
1	A	320	ALA
1	B	63	SER
1	B	339	LYS
1	C	29	LEU
1	C	59	GLY
1	C	222	PHE
1	D	30	ARG
1	D	32	ARG
1	D	63	SER
1	D	281	ASN
1	A	12	ARG
1	A	35	VAL
1	A	58	ALA
1	A	95	THR
1	B	78	ASN
1	B	321	GLU
1	C	35	VAL
1	C	152	MSE
1	C	159	VAL
1	C	321	GLU
1	C	338	LEU
1	D	78	ASN
1	A	60	ALA
1	D	35	VAL
1	D	36	SER

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Mol	Chain	Res	Type
1	A	21	SER
1	B	152	MSE
1	D	57	ILE
1	C	156	GLY

5.3.2　Protein sidechains　ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/264 (102%)	254 (94%)	15 (6%)	21	24
1	B	269/264 (102%)	262 (97%)	7 (3%)	46	56
1	C	269/264 (102%)	261 (97%)	8 (3%)	41	50
1	D	271/264 (103%)	261 (96%)	10 (4%)	34	43
All	All	1078/1056 (102%)	1038 (96%)	40 (4%)	34	43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	23	MSE
1	A	24	THR
1	A	27	ARG
1	A	30	ARG
1	A	56	LYS
1	A	94	ASP
1	A	142	ASP
1	A	155	ASP
1	A	192	LYS
1	A	237	GLN
1	A	255	MSE
1	A	286	LEU
1	A	306	LYS
1	A	321	GLU
1	B	39	THR
1	B	78	ASN

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Mol	Chain	Res	Type
1	B	204	GLU
1	B	277	LEU
1	B	284	GLU
1	B	286	LEU
1	B	315	LEU
1	C	169	ARG
1	C	173	GLU
1	C	220	ARG
1	C	234	GLU
1	C	255	MSE
1	C	286	LEU
1	C	300	ARG
1	C	336	ASP
1	D	32	ARG
1	D	78	ASN
1	D	93	GLU
1	D	140	MSE
1	D	168	ARG
1	D	194	PRO
1	D	220	ARG
1	D	285	LEU
1	D	315	LEU
1	D	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	89	ASN
1	B	64	ASN
1	B	89	ASN
1	B	98	GLN
1	C	64	ASN
1	C	176	GLN
1	D	98	GLN
1	D	281	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	320/344 (93%)	0.45	34 (10%)	6	10	22, 38, 107, 121	0
1	B	320/344 (93%)	0.27	13 (4%)	37	48	24, 43, 68, 88	0
1	C	320/344 (93%)	0.23	19 (5%)	22	31	19, 41, 75, 84	0
1	D	322/344 (93%)	0.20	19 (5%)	22	31	19, 34, 84, 113	0
All	All	1282/1376 (93%)	0.29	85 (6%)	18	26	19, 39, 83, 121	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	ALA	10.7
1	A	60	ALA	9.1
1	D	33	GLY	8.4
1	A	33	GLY	7.1
1	B	60	ALA	7.1
1	B	61	LEU	6.8
1	A	34	ASP	6.8
1	D	62	ALA	6.5
1	A	22	GLU	6.4
1	C	222	PHE	6.0
1	C	63	SER	5.9
1	A	95	THR	5.8
1	A	29	LEU	5.7
1	D	60	ALA	5.7
1	D	39	THR	5.3
1	D	34	ASP	5.2
1	C	62	ALA	5.1
1	D	31	ASN	5.0
1	D	38	ALA	5.0
1	A	28	VAL	4.8
1	A	30	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	61	LEU	4.6
1	C	60	ALA	4.6
1	D	63	SER	4.0
1	D	322	ILE	3.9
1	C	157	LYS	3.9
1	C	39	THR	3.9
1	D	59	GLY	3.7
1	D	58	ALA	3.6
1	A	325	ARG	3.6
1	D	29	LEU	3.5
1	C	64	ASN	3.5
1	A	61	LEU	3.5
1	A	10	THR	3.5
1	A	21	SER	3.5
1	C	194	PRO	3.5
1	D	40	ARG	3.5
1	D	32	ARG	3.4
1	A	37	ASP	3.4
1	A	16	GLU	3.3
1	C	225	GLY	3.2
1	D	287	GLN	3.1
1	B	63	SER	3.0
1	D	61	LEU	3.0
1	C	58	ALA	3.0
1	B	176	GLN	3.0
1	A	35	VAL	3.0
1	A	12	ARG	2.9
1	C	158	PRO	2.9
1	B	135	GLU	2.9
1	A	63	SER	2.9
1	B	320	ALA	2.8
1	A	20	VAL	2.7
1	A	42	ARG	2.7
1	A	40	ARG	2.7
1	A	49	GLU	2.6
1	A	41	ALA	2.6
1	A	39	THR	2.6
1	B	273	GLY	2.6
1	A	25	VAL	2.6
1	B	222	PHE	2.5
1	B	57	ILE	2.5
1	B	58	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	339	LYS	2.5
1	D	36	SER	2.5
1	A	24	THR	2.5
1	C	241	GLU	2.5
1	A	321	GLU	2.4
1	A	31	ASN	2.4
1	B	64	ASN	2.4
1	D	30	ARG	2.4
1	A	59	GLY	2.4
1	A	186	ILE	2.3
1	A	57	ILE	2.3
1	A	19	GLY	2.3
1	C	59	GLY	2.2
1	A	184	ARG	2.1
1	A	44	LEU	2.1
1	A	18	SER	2.1
1	C	221	GLU	2.1
1	C	37	ASP	2.1
1	C	11	LEU	2.1
1	D	12	ARG	2.0
1	C	191	THR	2.0
1	C	211	GLY	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.