Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 03:35 AM EST

PDB ID	:	3OPO
Title	:	Crystal structure of the membrane fusion protein CusB from Escherichia coli
Authors	:	Su, C.-C.
Deposited on	:	2010-09-01
Resolution	:	3.85 Å(reported)

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

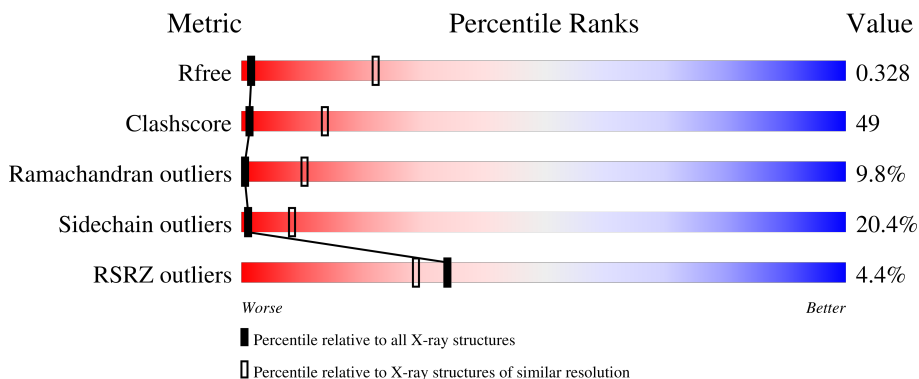|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.85 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		0.328
Clashscore		49
Ramachandran outliers		9.8%
Sidechain outliers		20.4%
RSRZ outliers		4.4%

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	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

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	413	2%　22%　36%　12%　•　28%
1	B	413	4%　22%　36%　12%　•　28%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AG	A	414	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4543 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.

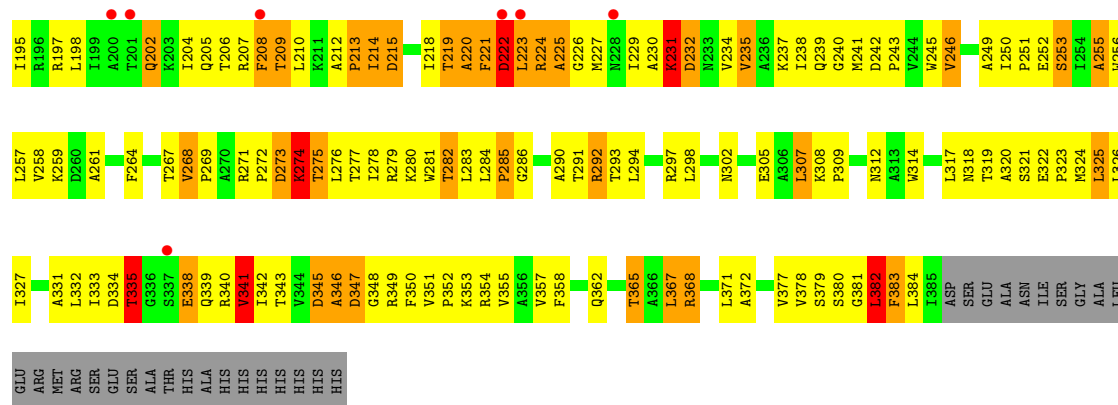- Molecule 1 is a protein called Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2267	1444	391	427	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	expression tag	UNP P77239
A	409	HIS	-	expression tag	UNP P77239
A	410	HIS	-	expression tag	UNP P77239
A	411	HIS	-	expression tag	UNP P77239
A	412	HIS	-	expression tag	UNP P77239
A	413	HIS	-	expression tag	UNP P77239
B	408	HIS	-	expression tag	UNP P77239
B	409	HIS	-	expression tag	UNP P77239
B	410	HIS	-	expression tag	UNP P77239
B	411	HIS	-	expression tag	UNP P77239
B	412	HIS	-	expression tag	UNP P77239
B	413	HIS	-	expression tag	UNP P77239

- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ag	0	0
			1	1		
2	B	1	Total	Ag	0	0
			1	1		

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: Cation efflux system protein cusB

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4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	84.80Å 114.68Å 259.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.31 – 3.85 39.31 – 3.85	Depositor EDS
% Data completeness (in resolution range)	90.9 (39.31-3.85) 98.8 (39.31-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 3.87Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.295 , 0.340 0.282 , 0.328	Depositor DCC
R_{free} test set	586 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å²)	159.3	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 239.3	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å²)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.04% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: AG

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	0.32	1/2306 (0.0%)	0.53	0/3142
1	B	0.27	0/2313	0.54	0/3152
All	All	0.30	1/4619 (0.0%)	0.53	0/6294

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CB-CG	5.26	1.62	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2267	0	2336	233	0
1	B	2274	0	2343	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4543	0	4679	449	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

All (449) 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:332:LEU:HA	1:A:341:VAL:HG11	1.32	1.08
1:A:117:ASN:HD21	1:A:243:PRO:HG2	1.21	1.01
1:A:122:ALA:HB3	1:A:214:ILE:HD12	1.49	0.94
1:A:106:PHE:CD2	1:B:253:SER:HA	2.06	0.89
1:A:249:ALA:HB1	1:A:293:THR:HG21	1.52	0.89
1:B:340:ARG:HA	1:B:355:VAL:HG22	1.54	0.88
1:A:255:ALA:O	1:A:258:VAL:HG12	1.73	0.87
1:A:343:THR:HB	1:A:351:VAL:HG13	1.56	0.87
1:A:150:LEU:HD11	1:A:212:ALA:HB2	1.56	0.87
1:A:340:ARG:HB2	1:A:353:LYS:O	1.75	0.86
1:A:94:VAL:HG13	1:A:381:GLY:HA2	1.56	0.85
1:A:154:THR:HG22	1:A:207:ARG:HB3	1.58	0.85
1:B:340:ARG:HB2	1:B:353:LYS:O	1.77	0.84
1:B:127:ARG:HD2	1:B:189:GLY:HA3	1.59	0.84
1:B:94:VAL:HG13	1:B:381:GLY:HA2	1.58	0.84
1:B:89:THR:HA	1:B:383:PHE:HE1	1.41	0.83
1:B:246:VAL:HG13	1:B:298:LEU:HB2	1.60	0.83
1:A:220:ALA:O	1:A:221:PHE:HB3	1.77	0.82
1:B:94:VAL:HG12	1:B:95:LYS:H	1.44	0.82
1:A:253:SER:HA	1:B:106:PHE:CD2	2.15	0.82
1:B:174:THR:HG23	1:B:177:GLN:HG2	1.60	0.82
1:B:103:PRO:HB3	1:B:321:SER:O	1.80	0.81
1:A:103:PRO:HB3	1:A:321:SER:O	1.81	0.81
1:A:324:MET:O	1:A:326:LEU:HD23	1.81	0.81
1:B:154:THR:HG22	1:B:207:ARG:HB3	1.63	0.80
1:B:220:ALA:O	1:B:221:PHE:HB3	1.80	0.80
1:A:132:ILE:HG22	1:A:227:MET:H	1.45	0.80
1:A:94:VAL:HG12	1:A:95:LYS:H	1.48	0.79
1:B:117:ASN:HD21	1:B:243:PRO:HG2	1.46	0.79
1:B:319:THR:HG22	1:B:320:ALA:H	1.46	0.78
1:B:89:THR:HA	1:B:383:PHE:CE1	2.19	0.78
1:A:219:THR:HG21	1:A:239:GLN:HG2	1.66	0.77
1:A:117:ASN:ND2	1:A:243:PRO:HG2	1.99	0.77
1:B:114:VAL:HB	1:B:309:PRO:HA	1.66	0.76
1:B:132:ILE:HG22	1:B:227:MET:H	1.48	0.76
1:A:278:ILE:HD11	1:A:298:LEU:HD22	1.65	0.76
1:A:132:ILE:HG12	1:A:133:ASP:N	2.02	0.75
1:A:281:TRP:HB3	1:A:298:LEU:HD21	1.70	0.74
1:A:202:GLN:HA	1:A:202:GLN:HE21	1.53	0.73
1:B:131:PHE:O	1:B:153:LEU:HB2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TRP:HE1	1:A:299:GLU:HG2	1.54	0.73
1:B:343:THR:HB	1:B:351:VAL:HG13	1.69	0.73
1:A:132:ILE:HG12	1:A:133:ASP:H	1.53	0.72
1:B:202:GLN:HE21	1:B:202:GLN:HA	1.52	0.72
1:B:120:GLN:HG3	1:B:240:GLY:HA3	1.72	0.72
1:A:242:ASP:HB3	1:A:243:PRO:HD3	1.72	0.72
1:B:341:VAL:HG13	1:B:342:ILE:N	2.04	0.72
1:B:147:GLY:HA2	1:B:212:ALA:O	1.90	0.71
1:B:162:GLN:HE22	1:B:205:GLN:HB2	1.57	0.70
1:A:112:ALA:HB1	1:A:246:VAL:HG23	1.74	0.70
1:B:112:ALA:HB1	1:B:246:VAL:HG23	1.74	0.70
1:B:145:GLN:O	1:B:146:LYS:HB2	1.90	0.70
1:A:332:LEU:HA	1:A:341:VAL:CG1	2.15	0.70
1:A:321:SER:HA	1:B:256:TRP:CE2	2.27	0.70
1:A:250:ILE:O	1:A:293:THR:HA	1.90	0.70
1:A:158:TRP:HE1	1:A:190:MET:HG3	1.56	0.69
1:B:132:ILE:HG23	1:B:226:GLY:HA2	1.73	0.69
1:A:147:GLY:HA2	1:A:212:ALA:O	1.93	0.69
1:A:128:ALA:HA	1:A:231:LYS:HA	1.75	0.69
1:A:355:VAL:HG11	1:A:371:LEU:HG	1.76	0.68
1:B:152:ASP:HA	1:B:209:THR:HA	1.75	0.68
1:B:255:ALA:O	1:B:258:VAL:HG12	1.93	0.68
1:A:128:ALA:HB3	1:A:158:TRP:HZ3	1.57	0.68
1:B:229:ILE:HG22	1:B:230:ALA:H	1.60	0.67
1:A:218:ILE:HD12	1:A:218:ILE:H	1.61	0.66
1:A:278:ILE:HD11	1:A:298:LEU:CD2	2.24	0.66
1:B:381:GLY:O	1:B:382:LEU:HB3	1.94	0.66
1:B:324:MET:O	1:B:326:LEU:CD2	2.44	0.66
1:B:126:ALA:O	1:B:232:ASP:HA	1.96	0.66
1:B:324:MET:O	1:B:326:LEU:HD22	1.96	0.66
1:A:97:ALA:O	1:A:376:LYS:HG3	1.96	0.66
1:A:229:ILE:HG22	1:A:230:ALA:H	1.60	0.66
1:A:340:ARG:HA	1:A:355:VAL:HG22	1.77	0.66
1:B:280:LYS:HG2	1:B:281:TRP:N	2.11	0.66
1:B:132:ILE:HG12	1:B:133:ASP:N	2.11	0.65
1:A:94:VAL:HG12	1:A:95:LYS:N	2.09	0.65
1:A:190:MET:SD	1:A:195:ILE:HG12	2.36	0.65
1:B:249:ALA:HB1	1:B:293:THR:HG21	1.78	0.65
1:B:278:ILE:HD11	1:B:298:LEU:HD13	1.78	0.64
1:A:357:VAL:HG23	1:B:285:PRO:HG2	1.78	0.64
1:A:368:ARG:O	1:A:368:ARG:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:O	1:B:293:THR:HA	1.97	0.64
1:A:145:GLN:O	1:A:146:LYS:HB2	1.96	0.64
1:B:327:ILE:HG13	1:B:365:THR:HG23	1.80	0.64
1:A:159:VAL:HA	1:A:162:GLN:CG	2.29	0.63
1:A:254:ILE:HG22	1:A:254:ILE:O	1.98	0.63
1:B:190:MET:SD	1:B:195:ILE:HG12	2.39	0.63
1:B:156:PRO:O	1:B:158:TRP:N	2.31	0.63
1:B:355:VAL:HG11	1:B:371:LEU:HG	1.81	0.63
1:A:144:VAL:HG12	1:A:218:ILE:HD11	1.80	0.62
1:A:256:TRP:CE2	1:B:321:SER:HA	2.34	0.62
1:B:268:VAL:HG23	1:B:271:ARG:O	1.98	0.62
1:B:94:VAL:HG12	1:B:95:LYS:N	2.13	0.62
1:A:355:VAL:HG12	1:A:370:GLY:HA3	1.80	0.62
1:B:274:LYS:H	1:B:274:LYS:HD2	1.65	0.62
1:A:244:VAL:HG12	1:A:245:TRP:N	2.15	0.61
1:A:317:LEU:HD12	1:A:318:ASN:H	1.66	0.61
1:A:210:LEU:O	1:A:210:LEU:HD12	2.01	0.61
1:B:220:ALA:O	1:B:221:PHE:CB	2.48	0.61
1:A:156:PRO:O	1:A:158:TRP:N	2.34	0.60
1:A:178:THR:O	1:A:181:ILE:HG22	2.01	0.60
1:A:244:VAL:HG12	1:A:245:TRP:H	1.66	0.60
1:B:297:ARG:O	1:B:298:LEU:HD23	2.02	0.60
1:A:220:ALA:O	1:A:221:PHE:CB	2.50	0.60
1:B:128:ALA:HA	1:B:231:LYS:HA	1.83	0.59
1:B:136:TYR:HD2	1:B:136:TYR:N	2.00	0.59
1:B:150:LEU:HD11	1:B:212:ALA:HB2	1.83	0.59
1:A:269:PRO:HD2	1:A:312:ASN:O	2.01	0.59
1:B:164:GLU:O	1:B:167:LEU:HG	2.02	0.59
1:A:258:VAL:HA	1:A:263:GLN:HE22	1.68	0.59
1:B:252:GLU:HA	1:B:255:ALA:HB2	1.85	0.59
1:B:302:ASN:OD1	1:B:305:GLU:HA	2.02	0.59
1:A:153:LEU:HD13	1:A:153:LEU:O	2.02	0.59
1:A:202:GLN:HE21	1:A:202:GLN:CA	2.15	0.59
1:B:202:GLN:HE21	1:B:202:GLN:CA	2.14	0.59
1:B:219:THR:HG21	1:B:239:GLN:HG2	1.85	0.59
1:A:132:ILE:CG1	1:A:133:ASP:H	2.15	0.59
1:A:308:LYS:HB3	1:A:309:PRO:HD2	1.85	0.59
1:A:122:ALA:CB	1:A:214:ILE:HD12	2.30	0.58
1:B:142:ASP:HB2	1:B:218:ILE:HD13	1.85	0.58
1:A:128:ALA:HB3	1:A:158:TRP:CZ3	2.37	0.58
1:B:152:ASP:OD1	1:B:152:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:HE2	1:A:178:THR:HB	1.68	0.58
1:A:321:SER:HA	1:B:256:TRP:CZ2	2.39	0.58
1:B:291:THR:O	1:B:293:THR:N	2.37	0.58
1:B:214:ILE:HG12	1:B:215:ASP:O	2.04	0.57
1:B:124:VAL:HG11	1:B:210:LEU:HD13	1.87	0.57
1:A:291:THR:O	1:A:293:THR:N	2.37	0.57
1:B:126:ALA:HB3	1:B:231:LYS:O	2.04	0.57
1:B:136:TYR:N	1:B:136:TYR:CD2	2.71	0.57
1:A:132:ILE:HG23	1:A:225:ALA:O	2.05	0.57
1:B:174:THR:CG2	1:B:177:GLN:HG2	2.34	0.57
1:A:142:ASP:H	1:A:218:ILE:HD13	1.69	0.57
1:A:162:GLN:HE22	1:A:205:GLN:HB2	1.68	0.57
1:B:122:ALA:HB3	1:B:214:ILE:HD12	1.85	0.57
1:B:319:THR:HG22	1:B:320:ALA:N	2.19	0.57
1:B:123:ILE:O	1:B:123:ILE:HD12	2.04	0.57
1:B:267:THR:HG23	1:B:314:TRP:HB2	1.85	0.57
1:A:256:TRP:CZ2	1:B:321:SER:HA	2.39	0.57
1:A:343:THR:OG1	1:A:353:LYS:HB2	2.05	0.57
1:B:134:LYS:O	1:B:135:VAL:HB	2.05	0.56
1:A:132:ILE:HD11	1:A:151:LEU:HD12	1.87	0.56
1:A:355:VAL:CG1	1:A:371:LEU:HG	2.35	0.56
1:B:191:PRO:HB2	1:B:194:ASP:HB2	1.87	0.56
1:A:134:LYS:O	1:A:135:VAL:HB	2.05	0.56
1:B:383:PHE:CD1	1:B:384:LEU:N	2.74	0.56
1:B:132:ILE:CG2	1:B:227:MET:H	2.18	0.56
1:B:339:GLN:HE22	1:B:357:VAL:HG22	1.69	0.56
1:B:368:ARG:HA	1:B:368:ARG:HH11	1.71	0.56
1:B:377:VAL:HG22	1:B:378:VAL:N	2.21	0.56
1:A:117:ASN:N	1:A:117:ASN:OD1	2.38	0.56
1:A:367:LEU:H	1:A:367:LEU:HD22	1.71	0.56
1:B:117:ASN:ND2	1:B:120:GLN:HB2	2.21	0.56
1:B:334:ASP:HB2	1:B:338:GLU:O	2.06	0.56
1:A:334:ASP:HB2	1:A:338:GLU:O	2.06	0.55
1:A:229:ILE:HG22	1:A:230:ALA:N	2.22	0.55
1:A:165:TYR:CE2	1:A:178:THR:HB	2.42	0.55
1:B:331:ALA:O	1:B:341:VAL:HG21	2.06	0.55
1:A:214:ILE:HD11	1:A:238:ILE:HB	1.88	0.55
1:B:135:VAL:HG11	1:B:224:ARG:HB2	1.88	0.55
1:A:132:ILE:CD1	1:A:151:LEU:HD12	2.36	0.55
1:A:345:ASP:O	1:A:347:ASP:N	2.40	0.55
1:B:132:ILE:CG1	1:B:133:ASP:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HG12	1:A:215:ASP:O	2.07	0.55
1:B:231:LYS:HB2	1:B:231:LYS:NZ	2.22	0.55
1:B:234:VAL:HG22	1:B:235:VAL:N	2.22	0.54
1:A:174:THR:CG2	1:A:177:GLN:HG2	2.37	0.54
1:A:317:LEU:HD12	1:A:318:ASN:N	2.22	0.54
1:B:146:LYS:CG	1:B:147:GLY:H	2.20	0.54
1:B:165:TYR:HB2	1:B:181:ILE:HG21	1.90	0.54
1:A:339:GLN:O	1:A:340:ARG:HB3	2.07	0.54
1:B:114:VAL:HG12	1:B:115:SER:H	1.72	0.54
1:A:331:ALA:O	1:A:341:VAL:HG11	2.08	0.54
1:A:244:VAL:HG21	1:A:307:LEU:HD11	1.89	0.54
1:B:343:THR:OG1	1:B:353:LYS:HB2	2.08	0.54
1:B:159:VAL:HA	1:B:162:GLN:HG2	1.90	0.53
1:A:359:GLN:HA	1:B:285:PRO:HB3	1.90	0.53
1:A:381:GLY:O	1:A:382:LEU:HB3	2.07	0.53
1:A:383:PHE:CG	1:A:384:LEU:N	2.75	0.53
1:A:319:THR:HG22	1:A:320:ALA:N	2.23	0.53
1:A:234:VAL:HG22	1:A:235:VAL:N	2.23	0.53
1:A:264:PHE:HE1	1:A:281:TRP:CD1	2.26	0.53
1:B:153:LEU:HD13	1:B:153:LEU:O	2.08	0.53
1:B:132:ILE:HD11	1:B:135:VAL:CG2	2.39	0.53
1:B:282:THR:HG23	1:B:297:ARG:HB3	1.91	0.53
1:B:135:VAL:HG21	1:B:224:ARG:HA	1.91	0.53
1:B:256:TRP:CD2	1:B:257:LEU:HD22	2.44	0.53
1:A:136:TYR:HB3	1:A:137:PRO:CD	2.40	0.52
1:A:368:ARG:HD3	1:A:368:ARG:C	2.29	0.52
1:B:278:ILE:CD1	1:B:298:LEU:HD13	2.38	0.52
1:A:117:ASN:HB3	1:A:245:TRP:CE2	2.44	0.52
1:A:91:ASN:ND2	1:A:93:GLY:H	2.08	0.52
1:A:324:MET:O	1:A:326:LEU:CD2	2.56	0.52
1:B:165:TYR:CE2	1:B:178:THR:HB	2.45	0.52
1:B:302:ASN:HD22	1:B:307:LEU:HG	1.74	0.52
1:A:237:LYS:HG2	1:A:238:ILE:N	2.25	0.52
1:A:327:ILE:HD13	1:A:367:LEU:HD21	1.91	0.52
1:B:95:LYS:HB3	1:B:380:SER:HB2	1.91	0.52
1:B:269:PRO:HD2	1:B:312:ASN:O	2.09	0.52
1:A:174:THR:HG23	1:A:177:GLN:HG2	1.91	0.52
1:B:229:ILE:HG22	1:B:230:ALA:N	2.24	0.52
1:A:268:VAL:HG23	1:A:271:ARG:O	2.10	0.52
1:B:136:TYR:HB3	1:B:137:PRO:CD	2.40	0.52
1:A:99:VAL:HG22	1:A:327:ILE:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ALA:HB1	1:A:293:THR:CG2	2.34	0.51
1:B:367:LEU:N	1:B:367:LEU:HD22	2.25	0.51
1:A:308:LYS:HD2	1:A:308:LYS:N	2.24	0.51
1:B:331:ALA:O	1:B:341:VAL:HG11	2.10	0.51
1:A:132:ILE:HG23	1:A:226:GLY:HA2	1.92	0.51
1:A:164:GLU:O	1:A:167:LEU:HG	2.10	0.51
1:B:136:TYR:HB3	1:B:137:PRO:HD2	1.93	0.51
1:B:168:LEU:HD12	1:B:173:GLY:HA3	1.91	0.51
1:A:126:ALA:O	1:A:232:ASP:HA	2.11	0.51
1:A:132:ILE:CG1	1:A:133:ASP:N	2.70	0.51
1:A:346:ALA:C	1:A:348:GLY:H	2.12	0.51
1:A:302:ASN:HD22	1:A:307:LEU:HG	1.74	0.51
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.26	0.51
1:B:284:LEU:O	1:B:286:GLY:N	2.41	0.51
1:B:122:ALA:CB	1:B:214:ILE:HD12	2.40	0.51
1:B:132:ILE:HG23	1:B:225:ALA:O	2.11	0.51
1:A:302:ASN:OD1	1:A:305:GLU:HA	2.10	0.50
1:A:136:TYR:HB3	1:A:137:PRO:HD2	1.92	0.50
1:B:152:ASP:CB	1:B:209:THR:HG23	2.41	0.50
1:A:121:TYR:C	1:A:121:TYR:CD2	2.84	0.50
1:A:284:LEU:C	1:A:286:GLY:H	2.15	0.50
1:B:355:VAL:CG1	1:B:371:LEU:HG	2.41	0.50
1:A:123:ILE:HD12	1:A:123:ILE:O	2.11	0.50
1:A:136:TYR:N	1:A:136:TYR:CD2	2.78	0.50
1:A:245:TRP:NE1	1:A:299:GLU:HG2	2.23	0.50
1:B:113:ASN:OD1	1:B:113:ASN:O	2.30	0.50
1:B:124:VAL:O	1:B:235:VAL:HG22	2.12	0.50
1:B:229:ILE:HD12	1:B:229:ILE:N	2.27	0.50
1:B:377:VAL:HG22	1:B:378:VAL:H	1.77	0.50
1:A:275:THR:HG21	1:A:277:THR:HG23	1.94	0.50
1:B:117:ASN:HB3	1:B:245:TRP:CE2	2.47	0.50
1:B:340:ARG:CB	1:B:354:ARG:HA	2.42	0.50
1:A:106:PHE:CE1	1:A:359:GLN:NE2	2.78	0.50
1:A:256:TRP:CD2	1:A:257:LEU:HD22	2.47	0.50
1:B:283:LEU:O	1:B:285:PRO:HD3	2.11	0.49
1:A:106:PHE:HE1	1:A:359:GLN:NE2	2.09	0.49
1:A:152:ASP:N	1:A:152:ASP:OD1	2.45	0.49
1:B:208:PHE:CD1	1:B:208:PHE:N	2.76	0.49
1:B:275:THR:HG22	1:B:276:LEU:H	1.76	0.49
1:B:341:VAL:HG13	1:B:342:ILE:H	1.75	0.49
1:A:266:LEU:HD22	1:A:315:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HG12	1:B:218:ILE:HD11	1.94	0.49
1:A:340:ARG:CB	1:A:354:ARG:HA	2.43	0.49
1:B:116:TYR:HE2	1:B:241:MET:HG2	1.78	0.49
1:B:159:VAL:HA	1:B:162:GLN:CG	2.43	0.49
1:A:267:THR:HG23	1:A:314:TRP:HB2	1.95	0.49
1:A:345:ASP:OD2	1:A:349:ARG:HG3	2.12	0.48
1:A:153:LEU:HD22	1:A:154:THR:N	2.28	0.48
1:A:215:ASP:OD1	1:A:215:ASP:N	2.41	0.48
1:B:219:THR:O	1:B:237:LYS:HB3	2.13	0.48
1:B:155:ILE:HG13	1:B:208:PHE:HE1	1.78	0.48
1:B:168:LEU:HB3	1:B:178:THR:HG22	1.94	0.48
1:B:205:GLN:OE1	1:B:205:GLN:HA	2.12	0.48
1:A:152:ASP:HA	1:A:209:THR:HA	1.95	0.48
1:A:230:ALA:O	1:A:233:ASN:HB2	2.13	0.48
1:B:145:GLN:O	1:B:146:LYS:CB	2.60	0.48
1:A:377:VAL:HG22	1:A:378:VAL:N	2.27	0.48
1:A:122:ALA:HB3	1:A:214:ILE:CD1	2.32	0.48
1:B:92:LEU:HA	1:B:94:VAL:HG23	1.94	0.48
1:B:115:SER:N	1:B:245:TRP:O	2.45	0.48
1:B:148:THR:HB	1:B:149:PRO:HD2	1.95	0.48
1:A:146:LYS:CG	1:A:147:GLY:H	2.25	0.48
1:A:331:ALA:HB2	1:A:379:SER:HB3	1.95	0.48
1:A:115:SER:N	1:A:245:TRP:O	2.47	0.48
1:B:117:ASN:C	1:B:119:TYR:H	2.16	0.48
1:B:146:LYS:HG2	1:B:147:GLY:N	2.28	0.48
1:B:150:LEU:N	1:B:150:LEU:HD12	2.29	0.48
1:B:219:THR:CG2	1:B:237:LYS:HD2	2.44	0.48
1:A:218:ILE:HD12	1:A:218:ILE:N	2.27	0.47
1:A:103:PRO:CB	1:A:321:SER:O	2.58	0.47
1:A:132:ILE:CG2	1:A:227:MET:H	2.21	0.47
1:A:135:VAL:HG11	1:A:224:ARG:HB2	1.94	0.47
1:B:197:ARG:HG2	1:B:205:GLN:NE2	2.28	0.47
1:A:244:VAL:O	1:A:299:GLU:HA	2.14	0.47
1:A:283:LEU:HD13	1:A:296:LEU:HD13	1.95	0.47
1:A:153:LEU:HD22	1:A:153:LEU:C	2.35	0.47
1:B:132:ILE:CG1	1:B:133:ASP:H	2.28	0.47
1:A:256:TRP:HE1	1:B:106:PHE:HE2	1.62	0.47
1:B:198:LEU:HD23	1:B:198:LEU:C	2.35	0.47
1:A:252:GLU:HA	1:A:255:ALA:HB2	1.96	0.47
1:B:339:GLN:O	1:B:340:ARG:HB3	2.14	0.47
1:B:342:ILE:HG13	1:B:378:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:HB3	1:A:309:PRO:CD	2.44	0.47
1:B:186:ARG:HA	1:B:190:MET:H	1.78	0.47
1:A:275:THR:HG22	1:A:276:LEU:N	2.30	0.47
1:A:92:LEU:O	1:A:92:LEU:HD22	2.15	0.47
1:B:383:PHE:CG	1:B:384:LEU:N	2.82	0.47
1:B:317:LEU:HD12	1:B:318:ASN:H	1.81	0.46
1:A:379:SER:O	1:A:380:SER:HB2	2.16	0.46
1:B:141:GLY:HA2	1:B:218:ILE:O	2.15	0.46
1:A:117:ASN:C	1:A:119:TYR:H	2.19	0.46
1:A:334:ASP:O	1:A:335:THR:HG23	2.15	0.46
1:B:178:THR:O	1:B:181:ILE:HG22	2.15	0.46
1:B:252:GLU:HG2	1:B:292:ARG:HB3	1.98	0.46
1:A:159:VAL:HG23	1:A:204:ILE:CD1	2.46	0.46
1:A:355:VAL:HA	1:A:370:GLY:HA3	1.97	0.46
1:B:158:TRP:HZ2	1:B:189:GLY:O	1.99	0.46
1:A:167:LEU:HD12	1:A:167:LEU:C	2.35	0.46
1:A:91:ASN:CG	1:A:92:LEU:N	2.70	0.46
1:A:131:PHE:O	1:A:153:LEU:HB2	2.16	0.46
1:A:219:THR:CG2	1:A:237:LYS:HD2	2.46	0.46
1:B:144:VAL:HG23	1:B:146:LYS:H	1.80	0.46
1:B:280:LYS:CG	1:B:281:TRP:N	2.79	0.46
1:A:319:THR:HG22	1:A:320:ALA:H	1.80	0.46
1:A:208:PHE:N	1:A:208:PHE:CD1	2.83	0.45
1:A:285:PRO:HB3	1:B:358:PHE:O	2.16	0.45
1:B:219:THR:O	1:B:220:ALA:HB3	2.16	0.45
1:B:351:VAL:HA	1:B:352:PRO:HD3	1.84	0.45
1:A:148:THR:HB	1:A:149:PRO:HD2	1.99	0.45
1:B:340:ARG:HB3	1:B:354:ARG:HA	1.99	0.45
1:A:152:ASP:CG	1:A:209:THR:HG23	2.37	0.45
1:B:157:ASP:O	1:B:158:TRP:C	2.55	0.45
1:A:132:ILE:HD11	1:A:135:VAL:CG2	2.47	0.45
1:A:94:VAL:HG13	1:A:381:GLY:CA	2.37	0.45
1:A:157:ASP:O	1:A:158:TRP:C	2.55	0.45
1:B:165:TYR:HE2	1:B:178:THR:HB	1.82	0.45
1:B:202:GLN:HA	1:B:202:GLN:NE2	2.26	0.45
1:A:284:LEU:O	1:A:286:GLY:N	2.49	0.45
1:B:121:TYR:C	1:B:121:TYR:CD2	2.90	0.45
1:B:158:TRP:HE1	1:B:190:MET:CG	2.30	0.45
1:B:237:LYS:HG2	1:B:238:ILE:N	2.31	0.45
1:B:334:ASP:O	1:B:335:THR:HG23	2.17	0.45
1:A:302:ASN:OD1	1:A:302:ASN:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.98	0.44
1:A:112:ALA:HB1	1:A:246:VAL:CG2	2.46	0.44
1:A:347:ASP:HB2	1:A:349:ARG:HG2	1.98	0.44
1:B:250:ILE:HD13	1:B:250:ILE:HA	1.75	0.44
1:B:224:ARG:O	1:B:225:ALA:HB3	2.18	0.44
1:A:278:ILE:CD1	1:A:298:LEU:HD22	2.41	0.44
1:B:146:LYS:CG	1:B:147:GLY:N	2.80	0.44
1:B:342:ILE:O	1:B:377:VAL:HG23	2.18	0.44
1:B:150:LEU:O	1:B:151:LEU:HB3	2.17	0.44
1:B:345:ASP:O	1:B:347:ASP:N	2.50	0.44
1:B:346:ALA:C	1:B:348:GLY:H	2.21	0.44
1:A:146:LYS:CG	1:A:147:GLY:N	2.81	0.44
1:A:283:LEU:O	1:A:285:PRO:HD3	2.17	0.44
1:B:99:VAL:HG22	1:B:327:ILE:HG22	2.00	0.44
1:B:112:ALA:HB1	1:B:246:VAL:CG2	2.45	0.43
1:A:254:ILE:O	1:A:254:ILE:CG2	2.65	0.43
1:B:132:ILE:CG2	1:B:227:MET:N	2.82	0.43
1:A:168:LEU:C	1:A:170:GLU:H	2.21	0.43
1:A:288:ASP:OD2	1:A:290:ALA:HB3	2.18	0.43
1:B:245:TRP:CZ2	1:B:297:ARG:HD3	2.54	0.43
1:B:342:ILE:HG21	1:B:378:VAL:HG12	2.01	0.43
1:B:308:LYS:H	1:B:308:LYS:HD2	1.83	0.43
1:B:371:LEU:HB3	1:B:372:ALA:H	1.71	0.43
1:B:273:ASP:HB3	1:B:274:LYS:HD2	2.00	0.43
1:A:342:ILE:HG21	1:A:378:VAL:HG12	2.01	0.43
1:B:91:ASN:ND2	1:B:93:GLY:H	2.17	0.43
1:B:156:PRO:O	1:B:159:VAL:HG23	2.19	0.43
1:B:347:ASP:HB2	1:B:349:ARG:HG2	2.01	0.43
1:A:94:VAL:CG1	1:A:95:LYS:H	2.25	0.43
1:B:210:LEU:HD12	1:B:210:LEU:C	2.39	0.43
1:B:261:ALA:HA	1:B:264:PHE:CD1	2.54	0.43
1:B:308:LYS:HD2	1:B:308:LYS:N	2.34	0.43
1:B:379:SER:O	1:B:380:SER:HB2	2.18	0.43
1:A:91:ASN:HD21	1:A:93:GLY:H	1.66	0.43
1:A:250:ILE:HD13	1:A:250:ILE:HA	1.86	0.43
1:A:252:GLU:HG3	1:A:253:SER:N	2.33	0.43
1:A:257:LEU:HB3	1:A:319:THR:HG23	2.00	0.43
1:A:275:THR:HG22	1:A:276:LEU:H	1.83	0.43
1:A:275:THR:C	1:A:276:LEU:HD22	2.39	0.43
1:A:134:LYS:O	1:A:135:VAL:CB	2.66	0.42
1:A:383:PHE:CD1	1:A:384:LEU:N	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:HB2	1:A:181:ILE:HG21	2.00	0.42
1:A:327:ILE:HG13	1:A:365:THR:HG23	2.00	0.42
1:B:134:LYS:O	1:B:135:VAL:CB	2.67	0.42
1:B:156:PRO:O	1:B:157:ASP:C	2.58	0.42
1:B:326:LEU:HD22	1:B:326:LEU:N	2.34	0.42
1:A:151:LEU:N	1:A:151:LEU:HD23	2.34	0.42
1:A:185:LEU:HD23	1:A:190:MET:SD	2.59	0.42
1:A:281:TRP:HB3	1:A:298:LEU:CD2	2.46	0.42
1:B:256:TRP:CE2	1:B:257:LEU:HD22	2.54	0.42
1:A:95:LYS:O	1:A:378:VAL:HG23	2.20	0.42
1:A:205:GLN:OE1	1:A:205:GLN:HA	2.18	0.42
1:A:283:LEU:HD21	1:A:294:LEU:HD12	2.01	0.42
1:A:377:VAL:HG22	1:A:378:VAL:H	1.84	0.42
1:A:144:VAL:HG23	1:A:146:LYS:H	1.85	0.42
1:A:256:TRP:CE3	1:B:322:GLU:HG2	2.55	0.42
1:A:256:TRP:CZ3	1:A:257:LEU:HD13	2.55	0.42
1:A:278:ILE:HG23	1:A:278:ILE:O	2.18	0.42
1:B:274:LYS:HB2	1:B:275:THR:H	1.45	0.42
1:B:275:THR:C	1:B:276:LEU:HD22	2.40	0.42
1:A:114:VAL:HG21	1:A:311:MET:HB2	2.02	0.42
1:A:142:ASP:HB2	1:A:218:ILE:HD13	2.01	0.42
1:A:339:GLN:HE22	1:A:357:VAL:HG22	1.84	0.42
1:B:168:LEU:CB	1:B:178:THR:HG22	2.50	0.42
1:B:250:ILE:HA	1:B:251:PRO:HD3	1.84	0.42
1:B:282:THR:OG1	1:B:283:LEU:N	2.53	0.42
1:B:333:ILE:HD12	1:B:334:ASP:H	1.84	0.42
1:A:136:TYR:N	1:A:136:TYR:HD2	2.17	0.42
1:A:229:ILE:N	1:A:229:ILE:HD12	2.34	0.42
1:B:223:LEU:HD23	1:B:223:LEU:H	1.85	0.42
1:B:275:THR:HG22	1:B:276:LEU:N	2.35	0.42
1:A:333:ILE:HG22	1:A:341:VAL:HG12	2.02	0.41
1:B:92:LEU:HD22	1:B:92:LEU:O	2.20	0.41
1:B:146:LYS:HG2	1:B:147:GLY:H	1.83	0.41
1:B:332:LEU:HA	1:B:341:VAL:HG21	2.02	0.41
1:A:144:VAL:HG12	1:A:218:ILE:CD1	2.49	0.41
1:A:214:ILE:HD13	1:A:214:ILE:H	1.85	0.41
1:A:279:ARG:HD3	1:A:301:ASP:OD1	2.20	0.41
1:A:308:LYS:H	1:A:311:MET:CE	2.33	0.41
1:B:213:PRO:HB2	1:B:214:ILE:HG23	2.02	0.41
1:A:202:GLN:HA	1:A:202:GLN:NE2	2.28	0.41
1:A:341:VAL:HB	1:A:342:ILE:H	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:HD23	1:B:223:LEU:N	2.35	0.41
1:A:244:VAL:CG1	1:A:245:TRP:N	2.83	0.41
1:B:102:GLY:O	1:B:323:PRO:HA	2.20	0.41
1:B:219:THR:HG23	1:B:237:LYS:HD2	2.02	0.41
1:B:367:LEU:HD22	1:B:367:LEU:H	1.84	0.41
1:A:308:LYS:HD2	1:A:308:LYS:H	1.85	0.41
1:A:340:ARG:HB3	1:A:354:ARG:HA	2.01	0.41
1:A:358:PHE:HB2	1:A:368:ARG:HB2	2.03	0.41
1:B:132:ILE:HA	1:B:153:LEU:HB2	2.03	0.41
1:A:142:ASP:N	1:A:218:ILE:HD13	2.33	0.41
1:A:156:PRO:O	1:A:157:ASP:C	2.59	0.41
1:A:283:LEU:HD11	1:A:294:LEU:HB2	2.02	0.41
1:B:116:TYR:CE2	1:B:241:MET:HG2	2.56	0.41
1:B:156:PRO:HB2	1:B:157:ASP:H	1.59	0.41
1:B:218:ILE:HA	1:B:238:ILE:HD13	2.02	0.41
1:B:223:LEU:H	1:B:223:LEU:CD2	2.31	0.41
1:A:155:ILE:HA	1:A:156:PRO:HD2	1.89	0.41
1:B:162:GLN:NE2	1:B:205:GLN:HB2	2.29	0.41
1:B:218:ILE:H	1:B:218:ILE:HD12	1.86	0.41
1:B:280:LYS:HG2	1:B:281:TRP:H	1.83	0.41
1:A:117:ASN:HA	1:A:245:TRP:CE3	2.56	0.41
1:A:256:TRP:CZ2	1:A:257:LEU:HD21	2.56	0.41
1:A:257:LEU:HD13	1:A:257:LEU:HA	1.89	0.41
1:B:167:LEU:C	1:B:167:LEU:HD12	2.41	0.41
1:B:250:ILE:O	1:B:294:LEU:N	2.52	0.41
1:A:150:LEU:O	1:A:151:LEU:HB3	2.21	0.40
1:A:218:ILE:H	1:A:218:ILE:CD1	2.32	0.40
1:A:304:ASP:OD1	1:A:306:ALA:HB2	2.20	0.40
1:A:344:VAL:HG22	1:A:350:PHE:HD1	1.86	0.40
1:B:153:LEU:CD2	1:B:155:ILE:HG12	2.52	0.40
1:A:153:LEU:HD13	1:A:153:LEU:C	2.41	0.40
1:B:222:ASP:OD1	1:B:223:LEU:HD23	2.21	0.40
1:B:353:LYS:HD2	1:B:353:LYS:HA	1.85	0.40
1:B:150:LEU:HB2	1:B:151:LEU:HD22	2.03	0.40
1:B:325:LEU:H	1:B:325:LEU:HG	1.59	0.40
1:A:107:ALA:O	1:A:108:GLN:HB2	2.21	0.40
1:A:159:VAL:HG23	1:A:204:ILE:HD13	2.03	0.40
1:A:238:ILE:HG22	1:A:239:GLN:N	2.37	0.40
1:B:322:GLU:HA	1:B:323:PRO:HD3	1.89	0.40
1:B:357:VAL:HG23	1:B:357:VAL:O	2.21	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	294/413 (71%)	220 (75%)	45 (15%)	29 (10%)	0	10
1	B	295/413 (71%)	218 (74%)	48 (16%)	29 (10%)	0	10
All	All	589/826 (71%)	438 (74%)	93 (16%)	58 (10%)	0	10

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	146	LYS
1	A	156	PRO
1	A	157	ASP
1	A	206	THR
1	A	274	LYS
1	A	279	ARG
1	A	290	ALA
1	A	292	ARG
1	A	335	THR
1	A	346	ALA
1	B	135	VAL
1	B	146	LYS
1	B	157	ASP
1	B	206	THR
1	B	221	PHE
1	B	279	ARG
1	B	290	ALA
1	B	292	ARG
1	B	335	THR
1	B	382	LEU
1	A	204	ILE
1	A	221	PHE
1	A	222	ASP
1	A	288	ASP

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Mol	Chain	Res	Type
1	A	341	VAL
1	A	382	LEU
1	B	108	GLN
1	B	156	PRO
1	B	222	ASP
1	B	231	LYS
1	B	255	ALA
1	B	274	LYS
1	B	341	VAL
1	B	346	ALA
1	A	108	GLN
1	A	220	ALA
1	A	231	LYS
1	A	272	PRO
1	A	273	ASP
1	A	347	ASP
1	B	225	ALA
1	B	232	ASP
1	B	273	ASP
1	A	213	PRO
1	B	220	ALA
1	A	232	ASP
1	A	285	PRO
1	A	340	ARG
1	B	172	GLY
1	B	204	ILE
1	B	213	PRO
1	B	347	ASP
1	A	225	ALA
1	B	118	GLU
1	B	272	PRO
1	B	285	PRO
1	A	243	PRO

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	242/338 (72%)	192 (79%)	50 (21%)	1	8
1	B	243/338 (72%)	194 (80%)	49 (20%)	1	9
All	All	485/676 (72%)	386 (80%)	99 (20%)	1	8

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	109	SER
1	A	113	ASN
1	A	114	VAL
1	A	116	TYR
1	A	121	TYR
1	A	124	VAL
1	A	136	TYR
1	A	142	ASP
1	A	144	VAL
1	A	148	THR
1	A	151	LEU
1	A	152	ASP
1	A	153	LEU
1	A	157	ASP
1	A	158	TRP
1	A	183	GLU
1	A	185	LEU
1	A	187	LEU
1	A	202	GLN
1	A	208	PHE
1	A	209	THR
1	A	214	ILE
1	A	215	ASP
1	A	219	THR
1	A	222	ASP
1	A	223	LEU
1	A	224	ARG
1	A	231	LYS
1	A	235	VAL
1	A	246	VAL
1	A	253	SER
1	A	259	LYS
1	A	268	VAL
1	A	277	THR

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Mol	Chain	Res	Type
1	A	282	THR
1	A	307	LEU
1	A	335	THR
1	A	338	GLU
1	A	345	ASP
1	A	350	PHE
1	A	351	VAL
1	A	362	GLN
1	A	365	THR
1	A	367	LEU
1	A	373	GLU
1	A	375	GLU
1	A	382	LEU
1	A	383	PHE
1	A	385	ILE
1	B	92	LEU
1	B	109	SER
1	B	121	TYR
1	B	136	TYR
1	B	138	LEU
1	B	142	ASP
1	B	144	VAL
1	B	148	THR
1	B	151	LEU
1	B	152	ASP
1	B	153	LEU
1	B	155	ILE
1	B	157	ASP
1	B	158	TRP
1	B	183	GLU
1	B	190	MET
1	B	194	ASP
1	B	202	GLN
1	B	208	PHE
1	B	209	THR
1	B	214	ILE
1	B	215	ASP
1	B	219	THR
1	B	222	ASP
1	B	223	LEU
1	B	224	ARG
1	B	231	LYS

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Mol	Chain	Res	Type
1	B	235	VAL
1	B	246	VAL
1	B	253	SER
1	B	259	LYS
1	B	268	VAL
1	B	274	LYS
1	B	275	THR
1	B	277	THR
1	B	282	THR
1	B	307	LEU
1	B	325	LEU
1	B	335	THR
1	B	338	GLU
1	B	341	VAL
1	B	345	ASP
1	B	350	PHE
1	B	362	GLN
1	B	365	THR
1	B	367	LEU
1	B	368	ARG
1	B	382	LEU
1	B	383	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	162	GLN
1	A	202	GLN
1	A	318	ASN
1	A	330	GLN
1	A	339	GLN
1	B	91	ASN
1	B	162	GLN
1	B	202	GLN
1	B	339	GLN

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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	296/413 (71%)	0.11	10 (3%)	45	37	112, 202, 318, 446	0
1	B	297/413 (71%)	0.28	16 (5%)	25	21	120, 214, 362, 581	0
All	All	593/826 (71%)	0.19	26 (4%)	34	29	112, 209, 343, 581	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	THR	7.5
1	A	90	GLN	3.4
1	B	200	ALA	3.3
1	B	158	TRP	3.1
1	B	223	LEU	2.8
1	A	211	LYS	2.8
1	B	89	THR	2.8
1	A	385	ILE	2.7
1	B	178	THR	2.7
1	B	228	ASN	2.6
1	B	124	VAL	2.6
1	B	222	ASP	2.6
1	A	129	ALA	2.6
1	A	91	ASN	2.5
1	A	236	ALA	2.4
1	A	157	ASP	2.4
1	A	340	ARG	2.4
1	B	337	SER	2.4
1	A	343	THR	2.3
1	B	165	TYR	2.2
1	B	172	GLY	2.2
1	B	193	ALA	2.2
1	A	221	PHE	2.1
1	B	208	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLN	2.1
1	B	116	TYR	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 ⓘ

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	AG	A	414	1/1	0.77	1.35	400,400,400,400	0
2	AG	B	414	1/1	0.80	1.07	268,268,268,268	0

6.5 Other polymers ⓘ

There are no such residues in this entry.