Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 08:07 pm GMT

PDB ID	:	7OJS
Title	:	Complex structure 2 of the Bacillus subtilis CdaA c-di-AMP cyclase domain (CdaACD) and the phosphoglucomutase GlmM short variant (GlmMF369)
Authors	:	Pathania, M.; Grundling, A.G.; Freemont, P.
Deposited on	:	2021-05-17
Resolution	:	4.20 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:

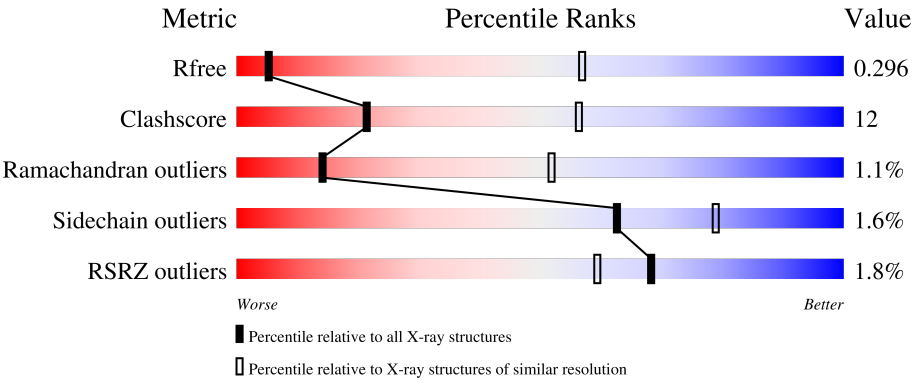
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	369	3% 70% 29%
1	B	369	5% 72% 27%
1	C	369	2% 72% 28%
1	F	369	% 73% 26%
1	G	369	2% 72% 27%

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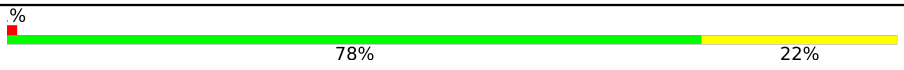
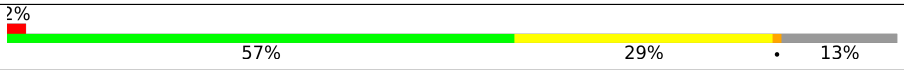
Mol	Chain	Length	Quality of chain
1	J	369	
2	D	167	
2	E	167	
2	H	167	
2	I	167	
2	K	167	
2	L	167	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23208 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 Phosphoglucosamine mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	368	Total	C	N	O	S	0	1	0
			2762	1731	464	553	14			
1	F	368	Total	C	N	O	S	0	1	0
			2762	1731	464	553	14			
1	A	368	Total	C	N	O	S	3	1	0
			2762	1731	464	553	14			
1	B	368	Total	C	N	O	S	0	1	0
			2762	1731	464	553	14			
1	G	368	Total	C	N	O	S	0	1	0
			2762	1731	464	553	14			
1	J	368	Total	C	N	O	S	3	1	0
			2762	1731	464	553	14			

- Molecule 2 is a protein called Cyclic di-AMP synthase CdaA.

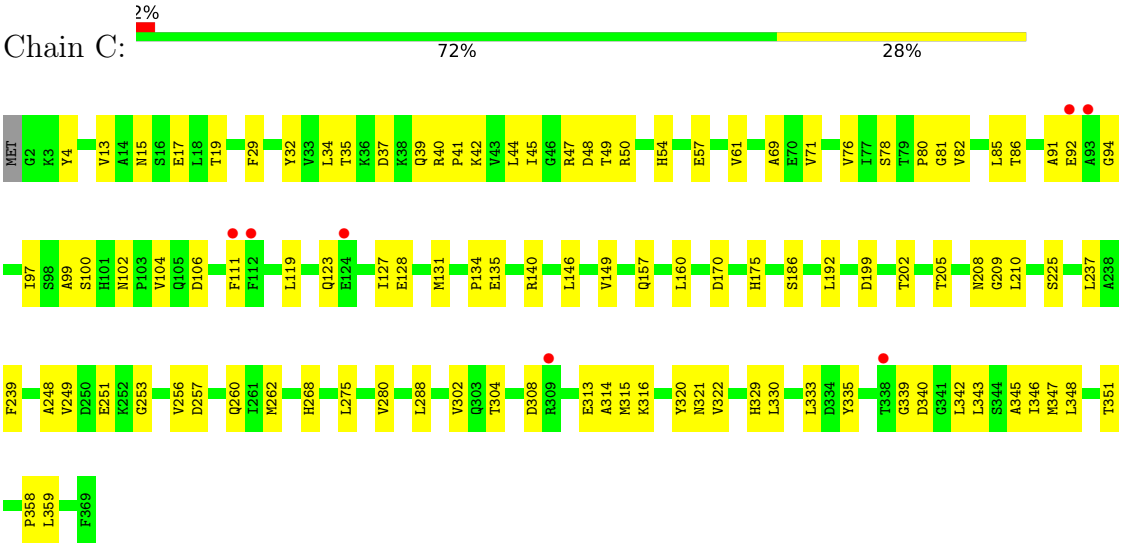
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	I	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	D	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	E	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	K	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	L	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			

3 Residue-property plots (i)

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

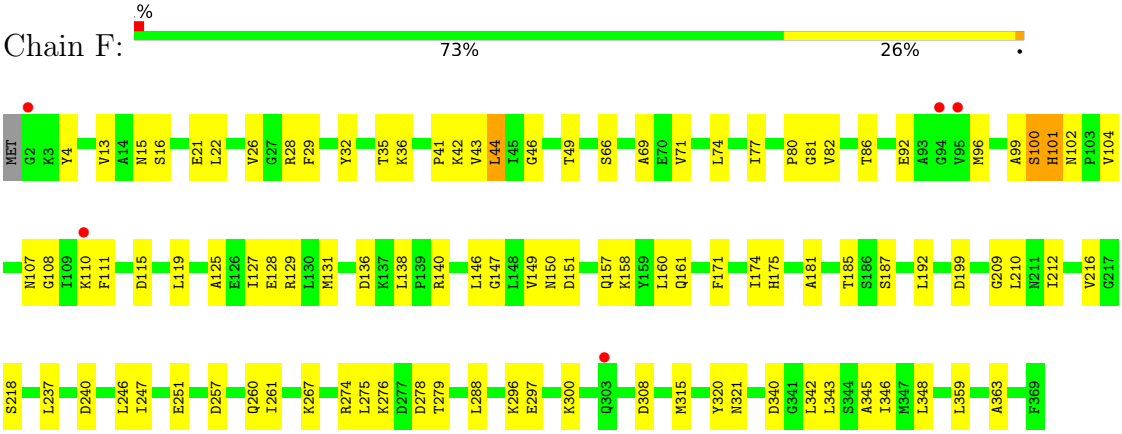
• Molecule 1: Phosphoglucosamine mutase

Chain C:



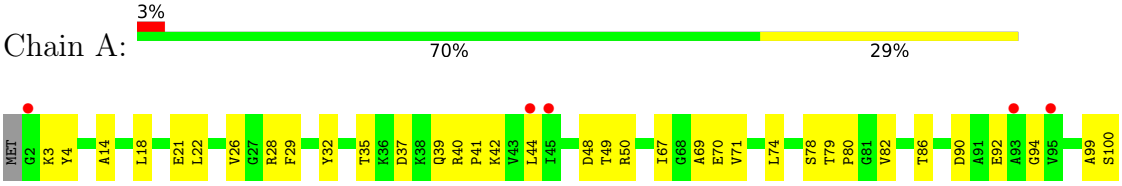
• Molecule 1: Phosphoglucosamine mutase

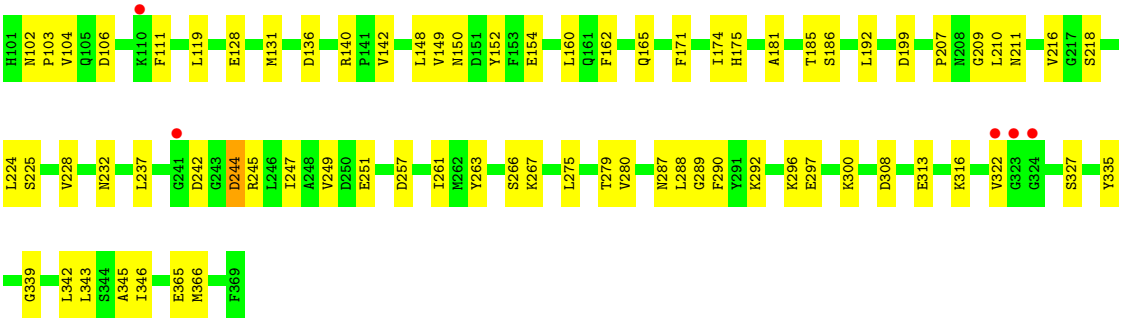
Chain F:



• Molecule 1: Phosphoglucosamine mutase

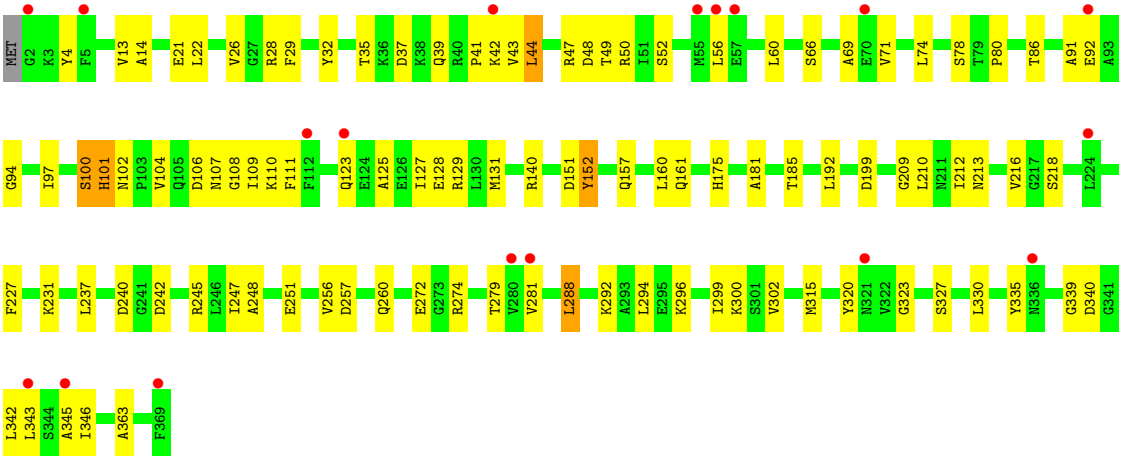
Chain A:





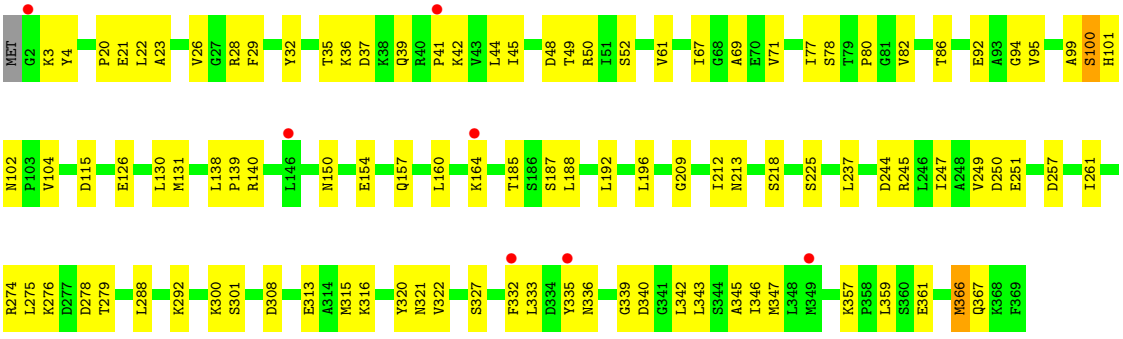
• Molecule 1: Phosphoglucosamine mutase

Chain B:



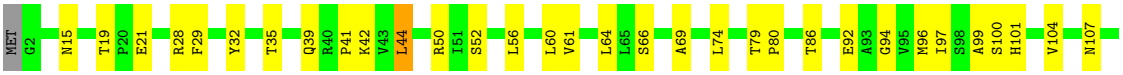
• Molecule 1: Phosphoglucosamine mutase

Chain G:

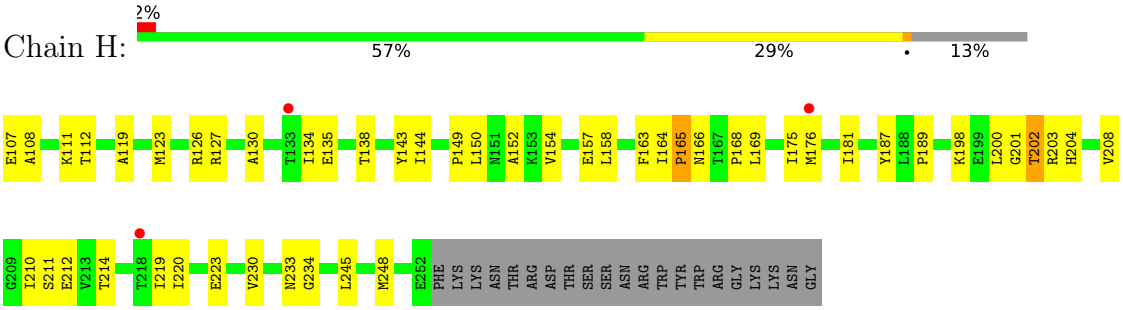


• Molecule 1: Phosphoglucosamine mutase

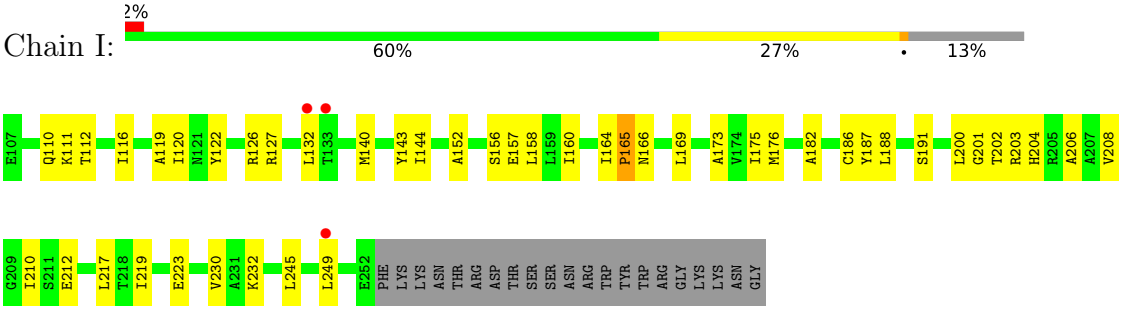
Chain J:



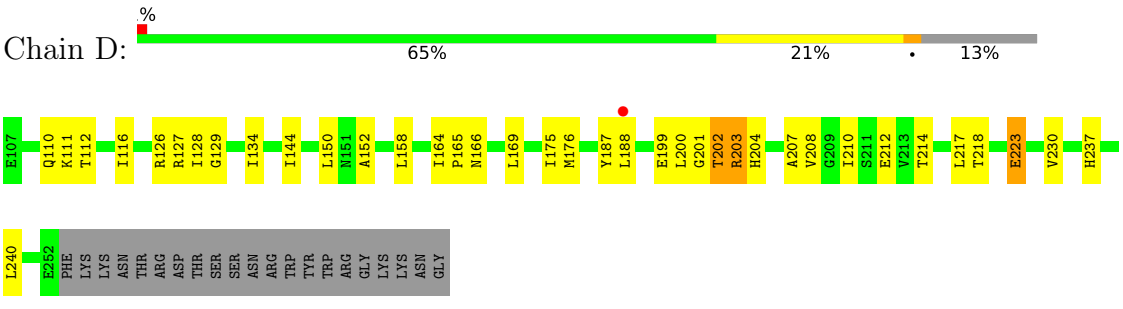
• Molecule 2: Cyclic di-AMP synthase CdaA



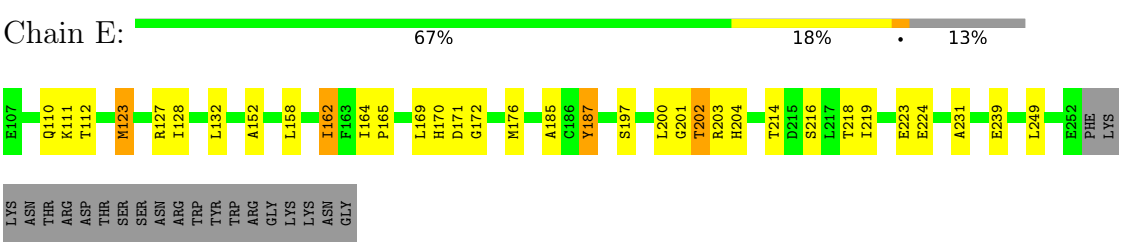
• Molecule 2: Cyclic di-AMP synthase CdaA



• Molecule 2: Cyclic di-AMP synthase CdaA

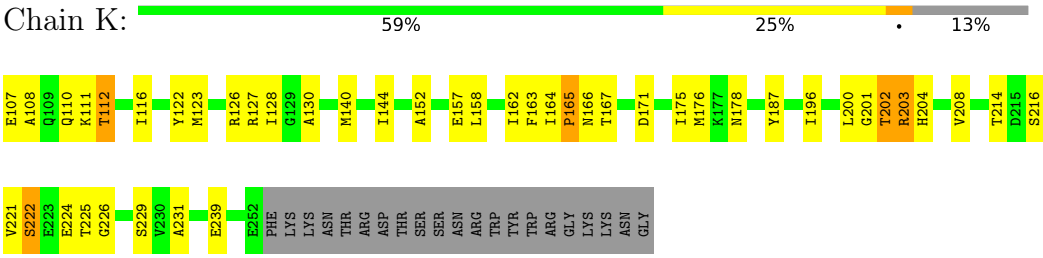


• Molecule 2: Cyclic di-AMP synthase CdaA



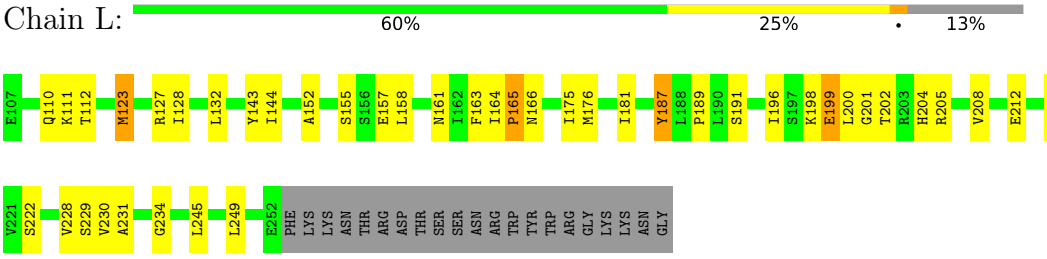
• Molecule 2: Cyclic di-AMP synthase CdaA

Chain K:



• Molecule 2: Cyclic di-AMP synthase CdaA

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.80Å 228.54Å 153.19Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	75.47 – 4.20 75.47 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (75.47-4.20) 99.2 (75.47-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 4.15Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.226 , 0.295 0.226 , 0.296	Depositor DCC
R_{free} test set	1497 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	103.1	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23208	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.26	0/2806	0.46	0/3781
1	B	0.26	0/2806	0.46	0/3781
1	C	0.26	0/2806	0.47	0/3781
1	F	0.26	0/2806	0.47	0/3781
1	G	0.26	0/2806	0.48	0/3781
1	J	0.26	0/2806	0.46	0/3781
2	D	0.26	0/1118	0.53	1/1512 (0.1%)
2	E	0.28	0/1118	0.51	0/1512
2	H	0.27	0/1118	0.54	1/1512 (0.1%)
2	I	0.30	0/1118	0.58	1/1512 (0.1%)
2	K	0.31	0/1118	0.58	0/1512
2	L	0.27	0/1118	0.53	0/1512
All	All	0.27	0/23544	0.49	3/31758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	187	TYR	C-N-CA	8.79	143.67	121.70
2	H	200	LEU	CA-CB-CG	5.41	127.75	115.30
2	D	200	LEU	CA-CB-CG	5.33	127.57	115.30

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	2762	0	2732	67	0
1	B	2762	0	2732	70	0
1	C	2762	0	2732	66	0
1	F	2762	0	2732	66	0
1	G	2762	0	2732	69	0
1	J	2762	0	2732	50	0
2	D	1106	0	1128	28	0
2	E	1106	0	1128	24	0
2	H	1106	0	1128	35	0
2	I	1106	0	1127	33	0
2	K	1106	0	1128	32	0
2	L	1106	0	1128	31	0
All	All	23208	0	23159	539	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 12.

All (539) 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)
2:H:123:MET:HE1	2:H:163:PHE:HB2	1.55	0.87
1:J:42:LYS:H	1:J:92:GLU:HG2	1.41	0.84
1:J:41:PRO:HD2	1:J:69:ALA:HA	1.60	0.81
2:L:144:ILE:HG12	2:L:175:ILE:HG21	1.63	0.79
2:L:200:LEU:HD23	2:L:222:SER:OG	1.83	0.78
1:A:111:PHE:HB3	1:A:119:LEU:HD13	1.66	0.78
1:B:315:MET:HA	1:B:320:TYR:HB2	1.64	0.78
1:A:86:THR:HG21	1:A:94:GLY:HA3	1.65	0.77
2:H:144:ILE:HG12	2:H:175:ILE:HG21	1.68	0.76
1:B:279:THR:HG22	1:B:300:LYS:HB2	1.67	0.76
2:L:220:ILE:HB	2:L:229:SER:HB2	1.68	0.75
1:A:104:VAL:HG21	1:A:210:LEU:HA	1.68	0.75
2:D:127:ARG:NH2	2:D:223:GLU:O	2.18	0.75
1:A:44:LEU:HD12	1:A:74:LEU:HD11	1.69	0.75
1:G:44:LEU:HD21	1:G:86:THR:HG22	1.66	0.75
1:C:104:VAL:HG21	1:C:210:LEU:HA	1.69	0.74
1:G:274:ARG:O	1:G:321:ASN:ND2	2.21	0.74
1:G:192:LEU:HD21	1:G:346:ILE:HD11	1.70	0.73
2:L:123:MET:HB3	2:L:128:ILE:HB	1.71	0.72
1:F:157:GLN:HA	1:F:160:LEU:HB3	1.71	0.72
2:K:127:ARG:HH21	2:K:224:GLU:HA	1.55	0.72
2:D:134:ILE:HA	2:D:176:MET:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ASP:O	2:H:126:ARG:NH1	2.23	0.71
1:F:279:THR:HG22	1:F:300:LYS:HB2	1.73	0.71
2:I:164:ILE:HG13	2:I:165:PRO:HD2	1.71	0.71
1:A:41:PRO:HD2	1:A:69:ALA:HA	1.72	0.70
2:H:169:LEU:HD11	2:I:158:LEU:HA	1.73	0.70
1:B:157:GLN:HA	1:B:160:LEU:HB3	1.72	0.70
1:F:104:VAL:HG23	1:F:212:ILE:HG22	1.73	0.70
1:J:151:ASP:O	2:K:126:ARG:NH1	2.24	0.70
2:I:144:ILE:HG12	2:I:175:ILE:HG21	1.73	0.70
1:C:61:VAL:HG13	1:C:71:VAL:HG11	1.74	0.69
1:A:335:TYR:HB2	1:A:343:LEU:HD21	1.75	0.69
1:F:44:LEU:HD12	1:F:74:LEU:HD11	1.75	0.69
1:G:160:LEU:HD11	1:G:192:LEU:HB2	1.75	0.69
1:J:248:ALA:HB3	1:J:256:VAL:HB	1.75	0.68
2:L:164:ILE:HG13	2:L:165:PRO:HD2	1.74	0.68
1:A:42:LYS:H	1:A:92:GLU:HG2	1.58	0.68
2:E:132:LEU:HD21	2:E:176:MET:HG3	1.76	0.67
1:J:44:LEU:HD12	1:J:74:LEU:HD11	1.74	0.67
2:H:111:LYS:O	2:H:112:THR:OG1	2.12	0.67
1:A:160:LEU:HD11	1:A:192:LEU:HB2	1.74	0.67
1:G:21:GLU:OE2	1:J:140:ARG:NH2	2.26	0.67
1:C:49:THR:O	1:C:209:GLY:HA2	1.94	0.67
2:D:144:ILE:HG12	2:D:175:ILE:HG21	1.76	0.67
2:I:127:ARG:NH2	2:I:223:GLU:O	2.28	0.67
2:H:164:ILE:HG13	2:H:165:PRO:HD2	1.76	0.66
1:F:42:LYS:H	1:F:92:GLU:HG2	1.60	0.66
1:J:192:LEU:HD21	1:J:346:ILE:HD11	1.75	0.66
2:D:150:LEU:HD22	2:E:158:LEU:HD22	1.77	0.66
1:G:42:LYS:H	1:G:92:GLU:HG2	1.60	0.66
2:K:225:THR:OG1	2:K:226:GLY:N	2.27	0.66
2:L:201:GLY:O	2:L:205:ARG:N	2.25	0.65
1:B:104:VAL:HG21	1:B:210:LEU:HA	1.77	0.65
1:G:279:THR:HG22	1:G:300:LYS:HB2	1.78	0.65
1:G:29:PHE:HD2	1:G:131:MET:HG2	1.62	0.64
1:C:78:SER:HB2	1:C:80:PRO:HD2	1.79	0.64
1:C:4:TYR:HD1	1:C:128:GLU:HG2	1.62	0.64
1:F:136:ASP:OD2	1:F:140:ARG:NH2	2.30	0.63
2:H:150:LEU:HD22	2:I:158:LEU:HD22	1.79	0.63
1:A:70:GLU:HG3	1:A:148:LEU:HD23	1.80	0.63
2:I:200:LEU:HD12	2:I:204:HIS:CD2	2.34	0.63
2:D:164:ILE:HG13	2:D:165:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:279:THR:HG22	1:J:300:LYS:HB2	1.80	0.63
1:G:50:ARG:NH2	1:G:99:ALA:O	2.32	0.63
1:A:225:SER:HA	1:A:249:VAL:HG11	1.79	0.62
1:A:192:LEU:HD21	1:A:346:ILE:HD11	1.81	0.62
2:H:157:GLU:OE2	2:H:157:GLU:N	2.32	0.62
2:H:168:PRO:HB2	2:I:157:GLU:HB3	1.81	0.62
1:J:86:THR:HG21	1:J:94:GLY:HA3	1.82	0.62
1:A:44:LEU:HD21	1:A:86:THR:HG22	1.80	0.61
1:B:86:THR:HG21	1:B:94:GLY:HA3	1.79	0.61
1:F:32:TYR:O	1:F:35:THR:HG22	2.00	0.61
1:F:218:SER:HB2	1:F:247:ILE:HG12	1.83	0.61
1:G:225:SER:HA	1:G:249:VAL:HG11	1.80	0.61
2:H:152:ALA:HB2	2:I:152:ALA:HB2	1.83	0.61
1:G:78:SER:HB2	1:G:80:PRO:HD2	1.83	0.61
2:H:119:ALA:O	2:H:123:MET:HG3	2.01	0.60
1:C:248:ALA:HB3	1:C:256:VAL:HB	1.83	0.60
1:B:335:TYR:HB2	1:B:343:LEU:HD21	1.82	0.60
1:G:80:PRO:HG3	1:G:339:GLY:O	2.01	0.60
1:C:35:THR:HA	1:C:41:PRO:HG3	1.83	0.60
2:K:200:LEU:HD12	2:K:204:HIS:CD2	2.36	0.60
1:B:181:ALA:HA	1:B:216:VAL:HG23	1.84	0.59
1:B:192:LEU:HD21	1:B:346:ILE:HD11	1.83	0.59
1:F:4:TYR:HD1	1:F:128:GLU:HG2	1.67	0.59
1:G:32:TYR:O	1:G:35:THR:HG22	2.03	0.59
1:C:313:GLU:HA	1:C:316:LYS:HD2	1.85	0.59
2:E:164:ILE:HG13	2:E:165:PRO:HD2	1.84	0.59
1:J:28:ARG:NH1	1:J:66:SER:O	2.36	0.59
1:J:32:TYR:O	1:J:35:THR:HG22	2.03	0.59
1:F:26:VAL:HA	1:F:131:MET:HE1	1.85	0.59
1:A:29:PHE:HD2	1:A:131:MET:HG2	1.67	0.59
1:A:279:THR:HG22	1:A:300:LYS:HB2	1.84	0.59
2:I:219:ILE:HD11	2:I:249:LEU:HD21	1.85	0.58
1:B:78:SER:HB2	1:B:80:PRO:HD2	1.83	0.58
2:L:164:ILE:O	2:L:166:ASN:N	2.36	0.58
2:K:220:ILE:HG22	2:K:221:VAL:H	1.68	0.58
1:B:32:TYR:O	1:B:35:THR:HG22	2.03	0.58
2:L:198:LYS:O	2:L:199:GLU:HB2	2.03	0.58
2:D:111:LYS:O	2:D:112:THR:OG1	2.14	0.58
1:F:315:MET:HA	1:F:320:TYR:HB2	1.84	0.58
1:A:48:ASP:OD2	1:A:50:ARG:NE	2.35	0.58
2:K:157:GLU:OE2	2:K:157:GLU:N	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:THR:HA	1:B:41:PRO:HG3	1.86	0.58
1:J:52:SER:OG	1:J:107:ASN:ND2	2.34	0.58
1:B:104:VAL:HG23	1:B:212:ILE:HG22	1.85	0.58
1:B:151:ASP:O	2:D:126:ARG:NH1	2.37	0.58
1:F:257:ASP:O	1:F:261:ILE:HG13	2.04	0.57
2:D:201:GLY:O	2:D:203:ARG:N	2.36	0.57
1:F:237:LEU:HD13	1:F:345:ALA:HB1	1.86	0.57
2:K:220:ILE:HB	2:K:229:SER:HB2	1.86	0.57
1:C:111:PHE:HB3	1:C:119:LEU:HD13	1.85	0.57
1:C:308:ASP:OD1	1:C:308:ASP:N	2.32	0.57
1:F:185:THR:HG22	1:F:342:LEU:HD11	1.87	0.57
2:D:217:LEU:HD11	2:D:230:VAL:HG22	1.86	0.57
1:C:157:GLN:HA	1:C:160:LEU:HB2	1.85	0.57
2:H:134:ILE:HA	2:H:176:MET:HB2	1.85	0.57
1:B:340:ASP:HB3	1:B:343:LEU:HB3	1.86	0.57
2:E:111:LYS:O	2:E:112:THR:OG1	2.22	0.57
2:E:127:ARG:NH2	2:E:223:GLU:O	2.37	0.57
2:L:218:THR:HB	2:L:231:ALA:HB3	1.86	0.56
1:F:49:THR:O	1:F:209:GLY:HA2	2.05	0.56
1:G:218:SER:HB2	1:G:247:ILE:HG12	1.87	0.56
1:B:107:ASN:OD1	1:B:108:GLY:N	2.35	0.56
1:J:104:VAL:HG21	1:J:210:LEU:HA	1.87	0.56
1:C:335:TYR:HB2	1:C:343:LEU:HD21	1.86	0.56
2:E:201:GLY:O	2:E:203:ARG:N	2.38	0.56
1:G:250:ASP:HA	1:G:359:LEU:HD23	1.87	0.56
1:C:29:PHE:HD2	1:C:131:MET:HG2	1.70	0.56
1:J:29:PHE:HD2	1:J:131:MET:HG2	1.71	0.56
1:C:44:LEU:HD21	1:C:86:THR:HG22	1.87	0.56
1:A:218:SER:HB2	1:A:247:ILE:HG12	1.87	0.56
1:G:48:ASP:OD2	1:G:50:ARG:NE	2.37	0.56
1:F:240:ASP:OD1	1:F:240:ASP:N	2.33	0.55
1:F:99:ALA:O	1:F:102:ASN:HB2	2.05	0.55
1:F:340:ASP:HB3	1:F:343:LEU:HB3	1.88	0.55
1:A:267:LYS:HG3	1:A:297:GLU:HG2	1.87	0.55
1:B:29:PHE:HD2	1:B:131:MET:HG2	1.71	0.55
1:B:212:ILE:HG12	1:B:213:ASN:ND2	2.21	0.55
1:G:251:GLU:OE1	1:G:251:GLU:N	2.38	0.55
1:C:262:MET:HG3	1:C:330:LEU:HD11	1.88	0.55
1:B:185:THR:HG22	1:B:342:LEU:HD11	1.88	0.55
2:K:111:LYS:O	2:K:112:THR:OG1	2.15	0.55
1:J:348:LEU:HD21	1:J:359:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:LYS:HB3	1:F:321:ASN:HB2	1.89	0.55
2:D:210:ILE:O	2:D:214:THR:OG1	2.22	0.55
1:J:163:LEU:O	1:J:166:THR:OG1	2.22	0.55
1:F:175:HIS:HA	1:F:199:ASP:HB2	1.87	0.54
2:D:158:LEU:HA	2:E:169:LEU:HD11	1.88	0.54
2:E:127:ARG:HH21	2:E:224:GLU:HA	1.70	0.54
1:G:41:PRO:HD2	1:G:69:ALA:HA	1.90	0.54
1:J:39:GLN:CD	1:J:39:GLN:H	2.11	0.54
2:H:201:GLY:HA2	2:H:204:HIS:HB2	1.90	0.54
1:A:313:GLU:HA	1:A:316:LYS:HD2	1.88	0.54
1:B:13:VAL:HA	1:B:106:ASP:HA	1.90	0.54
2:K:158:LEU:O	2:K:162:ILE:HG12	2.07	0.54
1:B:44:LEU:HD12	1:B:74:LEU:HD11	1.90	0.54
2:I:200:LEU:HD23	2:I:200:LEU:H	1.73	0.54
1:C:32:TYR:O	1:C:35:THR:HG22	2.08	0.53
2:I:200:LEU:HD12	2:I:204:HIS:CG	2.44	0.53
1:G:104:VAL:HG23	1:G:212:ILE:HG22	1.89	0.53
1:B:49:THR:O	1:B:209:GLY:HA2	2.09	0.53
1:G:22:LEU:O	1:G:26:VAL:HG23	2.08	0.53
1:F:82:VAL:O	1:F:86:THR:HG23	2.07	0.53
2:I:164:ILE:O	2:I:166:ASN:N	2.42	0.53
1:G:237:LEU:HD13	1:G:345:ALA:HB1	1.89	0.53
2:D:201:GLY:HA2	2:D:204:HIS:HB2	1.90	0.53
1:A:32:TYR:O	1:A:35:THR:HG22	2.09	0.53
1:C:45:ILE:HD11	1:C:97:ILE:HD11	1.91	0.53
2:H:210:ILE:O	2:H:214:THR:OG1	2.21	0.53
2:K:201:GLY:O	2:K:203:ARG:N	2.42	0.53
1:C:340:ASP:HB3	1:C:343:LEU:HB3	1.89	0.53
1:C:343:LEU:O	1:C:347:MET:HG2	2.09	0.53
1:G:29:PHE:CD2	1:G:131:MET:HG2	2.43	0.53
1:F:158:LYS:HE3	2:H:127:ARG:NH1	2.24	0.52
1:A:171:PHE:HB3	1:A:174:ILE:HD12	1.91	0.52
1:J:160:LEU:HD11	1:J:192:LEU:HB2	1.91	0.52
1:C:225:SER:HA	1:C:249:VAL:HG11	1.90	0.52
1:A:21:GLU:OE2	1:B:140:ARG:NH2	2.37	0.52
1:A:136:ASP:OD2	1:A:140:ARG:NH2	2.43	0.52
1:C:140:ARG:NH2	1:F:21:GLU:OE2	2.37	0.52
1:B:48:ASP:OD2	1:B:50:ARG:NE	2.43	0.52
1:J:237:LEU:HD13	1:J:345:ALA:HB1	1.91	0.52
1:G:313:GLU:HA	1:G:316:LYS:HD2	1.92	0.52
1:G:276:LYS:H	1:G:321:ASN:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:308:ASP:OD1	1:J:308:ASP:N	2.43	0.52
2:I:173:ALA:O	2:I:186:CYS:HB2	2.10	0.52
2:E:123:MET:HB3	2:E:128:ILE:HB	1.91	0.52
1:G:77:ILE:HG13	1:G:188:LEU:HD21	1.92	0.52
1:G:86:THR:HG21	1:G:94:GLY:HA3	1.91	0.52
2:L:201:GLY:O	2:L:204:HIS:N	2.43	0.52
1:C:225:SER:OG	1:C:253:GLY:O	2.22	0.51
1:A:207:PRO:HA	1:A:211:ASN:HD21	1.76	0.51
2:K:123:MET:HE1	2:K:163:PHE:HB2	1.92	0.51
1:F:260:GLN:NE2	1:F:363:ALA:HB1	2.25	0.51
2:I:157:GLU:HA	2:I:160:ILE:HD12	1.91	0.51
1:B:47:ARG:HB3	1:B:97:ILE:HB	1.92	0.51
1:A:99:ALA:O	1:A:102:ASN:HB2	2.11	0.51
1:G:39:GLN:CD	1:G:39:GLN:H	2.14	0.51
1:J:225:SER:OG	1:J:253:GLY:O	2.23	0.51
1:C:237:LEU:HD13	1:C:345:ALA:HB1	1.93	0.50
1:A:22:LEU:O	1:A:26:VAL:HG23	2.10	0.50
2:E:158:LEU:O	2:E:162:ILE:HG12	2.11	0.50
1:G:140:ARG:HD3	1:J:15:ASN:OD1	2.11	0.50
1:C:57:GLU:O	1:C:61:VAL:HG23	2.10	0.50
1:G:275:LEU:HG	1:G:278:ASP:HA	1.93	0.50
2:K:116:ILE:HD11	2:K:176:MET:SD	2.50	0.50
2:I:188:LEU:HD22	2:I:210:ILE:HG12	1.92	0.50
1:G:140:ARG:NH2	1:J:21:GLU:OE1	2.45	0.50
1:A:39:GLN:H	1:A:39:GLN:CD	2.15	0.50
1:A:82:VAL:O	1:A:86:THR:HG23	2.12	0.50
2:D:169:LEU:HD11	2:E:158:LEU:HA	1.92	0.50
1:C:280:VAL:HG13	1:C:322:VAL:HG12	1.94	0.50
1:G:333:LEU:HD23	1:G:336:ASN:O	2.11	0.50
2:L:219:ILE:HD11	2:L:249:LEU:HD21	1.94	0.50
1:A:237:LEU:HD13	1:A:345:ALA:HB1	1.94	0.50
1:G:42:LYS:H	1:G:92:GLU:CG	2.24	0.50
1:F:274:ARG:O	1:F:321:ASN:ND2	2.45	0.50
1:B:110:LYS:HD3	1:B:111:PHE:H	1.77	0.50
2:L:208:VAL:HG23	2:L:234:GLY:HA2	1.94	0.50
1:F:157:GLN:HA	1:F:160:LEU:CB	2.40	0.49
2:D:237:HIS:HB2	2:D:240:LEU:HD11	1.93	0.49
2:E:218:THR:HB	2:E:231:ALA:HB3	1.94	0.49
1:B:152:TYR:CZ	2:D:126:ARG:HB3	2.47	0.49
1:C:44:LEU:H	1:C:44:LEU:HD23	1.77	0.49
1:A:4:TYR:HD1	1:A:128:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:GLY:HA3	2:E:185:ALA:HA	1.94	0.49
1:F:111:PHE:HB3	1:F:119:LEU:HD13	1.93	0.49
1:C:40:ARG:NH2	1:C:146:LEU:O	2.45	0.49
1:B:161:GLN:HG2	2:D:166:ASN:HB2	1.93	0.49
2:E:197:SER:HB2	2:E:200:LEU:HD21	1.93	0.49
1:F:125:ALA:O	1:F:129:ARG:HG3	2.13	0.49
2:D:218:THR:O	2:D:230:VAL:HA	2.12	0.49
1:G:138:LEU:HD22	1:G:139:PRO:HD2	1.94	0.49
1:C:123:GLN:O	1:C:127:ILE:HG13	2.12	0.49
1:C:239:PHE:CE1	1:C:342:LEU:HG	2.47	0.49
1:C:304:THR:HG21	1:C:314:ALA:HB2	1.94	0.49
1:A:40:ARG:HH12	1:A:148:LEU:HB2	1.77	0.49
1:G:100:SER:O	1:G:102:ASN:N	2.46	0.49
2:K:222:SER:OG	2:K:226:GLY:N	2.46	0.49
1:F:171:PHE:HB3	1:F:174:ILE:HD12	1.95	0.49
1:A:342:LEU:H	1:A:342:LEU:HD12	1.78	0.49
1:C:4:TYR:CD1	1:C:128:GLU:HG2	2.47	0.49
2:H:211:SER:HB2	2:H:233:ASN:H	1.78	0.49
1:G:308:ASP:OD1	1:G:308:ASP:N	2.46	0.49
2:L:111:LYS:O	2:L:112:THR:OG1	2.22	0.49
2:L:228:VAL:HG11	2:L:245:LEU:HD22	1.95	0.49
1:G:82:VAL:O	1:G:86:THR:HG23	2.13	0.48
1:J:35:THR:HA	1:J:41:PRO:HG3	1.94	0.48
2:L:196:ILE:HD13	2:L:205:ARG:HG2	1.95	0.48
1:A:251:GLU:OE1	1:A:251:GLU:N	2.31	0.48
1:C:348:LEU:HD21	1:C:359:LEU:HD13	1.94	0.48
1:A:289:GLY:HA2	1:A:292:LYS:HB2	1.95	0.48
1:C:192:LEU:HD21	1:C:346:ILE:HD11	1.95	0.48
1:A:49:THR:O	1:A:209:GLY:HA2	2.14	0.48
1:C:48:ASP:OD2	1:C:50:ARG:NE	2.46	0.48
1:F:28:ARG:NH1	1:F:66:SER:O	2.46	0.48
1:J:79:THR:HG23	1:J:96:MET:HG2	1.95	0.48
1:C:315:MET:HB3	1:C:333:LEU:HD12	1.96	0.48
2:I:219:ILE:HD13	2:I:245:LEU:HD11	1.96	0.48
1:A:86:THR:CG2	1:A:94:GLY:HA3	2.39	0.48
1:B:80:PRO:HG3	1:B:339:GLY:O	2.14	0.48
2:L:123:MET:O	2:L:127:ARG:N	2.47	0.48
1:C:42:LYS:O	1:C:91:ALA:HB1	2.14	0.48
2:H:149:PRO:O	2:H:150:LEU:HD23	2.14	0.48
1:G:340:ASP:HB3	1:G:343:LEU:HB3	1.96	0.48
1:G:343:LEU:O	1:G:347:MET:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:132:LEU:HD21	2:L:176:MET:HG3	1.94	0.47
2:I:116:ILE:HD11	2:I:176:MET:CE	2.44	0.47
2:D:208:VAL:O	2:D:212:GLU:HG3	2.14	0.47
1:C:39:GLN:H	1:C:39:GLN:CD	2.11	0.47
1:A:175:HIS:HA	1:A:199:ASP:HB2	1.94	0.47
1:B:237:LEU:HD13	1:B:345:ALA:HB1	1.95	0.47
1:C:17:GLU:O	1:C:19:THR:HG23	2.14	0.47
2:H:230:VAL:HG11	2:H:248:MET:SD	2.54	0.47
1:B:21:GLU:OE1	1:B:21:GLU:N	2.38	0.47
2:I:204:HIS:O	2:I:208:VAL:HG12	2.15	0.47
1:A:154:GLU:HG2	2:E:187:TYR:CE1	2.49	0.47
1:J:251:GLU:OE1	1:J:251:GLU:N	2.47	0.47
1:A:162:PHE:O	1:A:165:GLN:HG3	2.14	0.47
1:B:157:GLN:HE22	2:E:164:ILE:HG12	1.78	0.47
1:B:247:ILE:HD12	1:B:257:ASP:HA	1.97	0.47
2:D:207:ALA:O	2:D:210:ILE:HG22	2.14	0.47
1:G:321:ASN:HB3	1:G:322:VAL:HG23	1.96	0.47
1:J:50:ARG:NH2	1:J:99:ALA:O	2.48	0.47
1:C:175:HIS:HA	1:C:199:ASP:HB2	1.96	0.47
1:B:41:PRO:HD2	1:B:69:ALA:HA	1.96	0.47
1:C:257:ASP:OD1	1:C:260:GLN:HG3	2.15	0.47
1:A:29:PHE:CD2	1:A:131:MET:HG2	2.50	0.47
1:B:294:LEU:HD22	1:B:299:ILE:HB	1.97	0.47
2:K:218:THR:HB	2:K:231:ALA:HB3	1.96	0.47
2:I:208:VAL:O	2:I:212:GLU:HG3	2.15	0.46
1:B:110:LYS:HD3	1:B:111:PHE:N	2.30	0.46
1:B:242:ASP:OD1	1:B:242:ASP:N	2.49	0.46
1:G:157:GLN:HA	1:G:160:LEU:HB3	1.97	0.46
2:K:152:ALA:HB2	2:L:152:ALA:HB2	1.97	0.46
1:F:308:ASP:OD1	1:F:308:ASP:N	2.36	0.46
1:B:60:LEU:HD21	1:B:109:ILE:HD13	1.97	0.46
2:E:170:HIS:O	2:E:172:GLY:N	2.48	0.46
1:A:28:ARG:NH1	1:A:67:ILE:HG23	2.31	0.46
1:C:50:ARG:NH2	1:C:99:ALA:O	2.48	0.46
1:F:36:LYS:HA	1:F:36:LYS:HD3	1.53	0.46
1:F:41:PRO:HD2	1:F:69:ALA:HA	1.98	0.46
2:H:130:ALA:O	2:H:220:ILE:HA	2.15	0.46
1:A:266:SER:HB2	1:A:275:LEU:HD22	1.98	0.46
1:J:283:THR:HG21	1:J:325:GLU:HG2	1.97	0.46
2:H:204:HIS:O	2:H:208:VAL:HG12	2.15	0.46
2:K:123:MET:HE1	2:K:130:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ASN:OD1	1:F:108:GLY:N	2.46	0.46
2:H:230:VAL:HG21	2:H:248:MET:SD	2.56	0.46
1:A:279:THR:HG22	1:A:300:LYS:HD2	1.98	0.46
1:G:4:TYR:CE2	1:G:22:LEU:HD21	2.50	0.46
1:F:43:VAL:O	1:F:71:VAL:HA	2.15	0.46
2:H:154:VAL:HG22	2:H:181:ILE:HG12	1.97	0.46
2:H:201:GLY:O	2:H:203:ARG:N	2.48	0.46
1:F:181:ALA:HA	1:F:216:VAL:HG23	1.98	0.46
2:D:152:ALA:HB2	2:E:152:ALA:HB2	1.97	0.46
2:E:200:LEU:HD12	2:E:204:HIS:CD2	2.51	0.46
1:G:357:LYS:HE3	1:G:361:GLU:OE2	2.16	0.46
2:K:126:ARG:HB2	2:K:128:ILE:HD11	1.98	0.46
1:F:251:GLU:OE1	1:F:251:GLU:N	2.48	0.46
2:H:219:ILE:HD13	2:H:245:LEU:HD11	1.97	0.46
1:B:302:VAL:HG21	1:B:320:TYR:CE2	2.51	0.46
1:J:218:SER:HB2	1:J:247:ILE:HG12	1.97	0.45
2:L:158:LEU:HD23	2:L:181:ILE:HD12	1.98	0.45
2:L:217:LEU:HD11	2:L:230:VAL:HG22	1.98	0.45
1:F:127:ILE:O	1:F:131:MET:HG3	2.16	0.45
1:A:224:LEU:O	1:A:228:VAL:HG23	2.16	0.45
1:J:227:PHE:CE1	1:J:231:LYS:HG3	2.51	0.45
2:K:167:THR:HB	2:L:161:ASN:OD1	2.15	0.45
1:C:302:VAL:HG21	1:C:320:TYR:HE2	1.81	0.45
2:H:127:ARG:NH2	2:H:223:GLU:O	2.49	0.45
2:H:138:THR:HG21	2:H:214:THR:HG22	1.98	0.45
2:H:158:LEU:HA	2:I:169:LEU:HD11	1.97	0.45
2:I:175:ILE:HG22	2:I:182:ALA:HB3	1.99	0.45
1:G:36:LYS:HD3	1:G:36:LYS:HA	1.57	0.45
1:C:175:HIS:HD2	1:C:199:ASP:O	2.00	0.45
1:F:150:ASN:N	1:F:150:ASN:OD1	2.50	0.45
1:F:275:LEU:HG	1:F:278:ASP:HA	1.98	0.45
1:B:28:ARG:NH1	1:B:66:SER:O	2.49	0.45
1:A:232:ASN:O	1:A:232:ASN:ND2	2.49	0.45
2:I:116:ILE:O	2:I:120:ILE:HG12	2.17	0.45
1:A:245:ARG:HD3	1:A:327:SER:HB3	1.97	0.45
2:E:219:ILE:HD11	2:E:249:LEU:HD21	1.97	0.45
1:G:3:LYS:HD2	1:G:3:LYS:HA	1.84	0.45
1:G:45:ILE:HG13	1:G:95:VAL:HB	1.99	0.45
1:G:245:ARG:HD3	1:G:327:SER:O	2.17	0.45
2:I:122:TYR:O	2:I:126:ARG:HG3	2.17	0.45
2:I:188:LEU:HB2	2:I:206:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:O	1:A:149:VAL:HA	2.17	0.45
1:A:257:ASP:O	1:A:261:ILE:HG13	2.16	0.45
1:J:60:LEU:HD12	1:J:97:ILE:HD11	1.98	0.45
1:C:34:LEU:HD11	1:C:119:LEU:HD21	1.98	0.45
1:F:138:LEU:HD23	1:F:138:LEU:HA	1.80	0.45
1:F:161:GLN:HG2	2:H:166:ASN:HB2	1.98	0.45
1:B:43:VAL:O	1:B:71:VAL:HA	2.17	0.45
2:D:126:ARG:HB2	2:D:128:ILE:HD11	1.97	0.45
1:C:81:GLY:O	1:C:85:LEU:HG	2.17	0.45
1:C:268:HIS:HB2	1:C:351:THR:HG23	1.99	0.45
1:F:44:LEU:HD21	1:F:86:THR:HA	1.98	0.45
1:F:115:ASP:N	1:F:115:ASP:OD1	2.48	0.45
1:F:246:LEU:O	1:F:247:ILE:HD13	2.17	0.45
1:F:348:LEU:HD21	1:F:359:LEU:HD13	1.99	0.45
1:G:292:LYS:HA	1:G:292:LYS:HD3	1.79	0.45
2:L:123:MET:CE	2:L:163:PHE:HB2	2.48	0.45
1:C:251:GLU:OE2	1:C:358:PRO:HB2	2.17	0.44
1:A:152:TYR:CE1	1:A:154:GLU:HB2	2.52	0.44
1:B:175:HIS:HA	1:B:199:ASP:HB2	1.98	0.44
1:B:248:ALA:HB3	1:B:256:VAL:HB	1.98	0.44
1:G:154:GLU:HG2	2:L:187:TYR:CZ	2.51	0.44
2:K:214:THR:C	2:K:216:SER:H	2.20	0.44
1:C:302:VAL:HG21	1:C:320:TYR:CE2	2.53	0.44
1:G:44:LEU:CD2	1:G:86:THR:HG22	2.43	0.44
1:C:42:LYS:H	1:C:92:GLU:HG2	1.83	0.44
1:C:86:THR:HG21	1:C:94:GLY:HA3	2.00	0.44
1:B:4:TYR:HD1	1:B:128:GLU:HG2	1.81	0.44
1:J:29:PHE:CD2	1:J:131:MET:HG2	2.49	0.44
2:K:196:ILE:HD11	2:K:208:VAL:HG11	1.98	0.44
1:C:71:VAL:O	1:C:149:VAL:HA	2.18	0.44
1:A:142:VAL:HG23	1:B:14:ALA:O	2.17	0.44
1:G:212:ILE:HG12	1:G:213:ASN:ND2	2.32	0.44
1:J:52:SER:O	1:J:56:LEU:HG	2.18	0.44
1:J:154:GLU:O	1:J:157:GLN:HG2	2.17	0.44
1:F:77:ILE:HD11	1:F:81:GLY:HA3	1.99	0.44
1:J:157:GLN:HA	1:J:160:LEU:HB3	1.99	0.44
1:C:329:HIS:CE1	1:C:339:GLY:HA3	2.53	0.44
1:B:260:GLN:HE21	1:B:363:ALA:HB1	1.83	0.44
1:G:126:GLU:O	1:G:130:LEU:HG	2.18	0.44
1:C:29:PHE:CD2	1:C:131:MET:HG2	2.50	0.44
2:H:158:LEU:HD23	2:H:181:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:LYS:O	2:I:112:THR:OG1	2.26	0.44
1:B:218:SER:OG	1:B:240:ASP:HB3	2.17	0.44
1:J:257:ASP:O	1:J:261:ILE:HG13	2.17	0.44
1:B:26:VAL:HG22	1:B:131:MET:HE1	2.00	0.44
1:B:245:ARG:HD3	1:B:327:SER:O	2.17	0.44
2:D:188:LEU:HD22	2:D:210:ILE:HD13	1.99	0.44
1:G:49:THR:O	1:G:209:GLY:HA2	2.17	0.44
2:K:128:ILE:HG23	2:K:165:PRO:HD3	1.99	0.44
2:L:200:LEU:HD12	2:L:200:LEU:HA	1.84	0.44
1:C:47:ARG:O	1:C:76:VAL:HA	2.18	0.44
2:H:201:GLY:C	2:H:202:THR:HG1	2.19	0.44
2:I:132:LEU:HD21	2:I:176:MET:HG3	2.00	0.44
1:B:42:LYS:H	1:B:92:GLU:HG2	1.82	0.44
1:J:250:ASP:HA	1:J:359:LEU:HD23	1.99	0.43
2:K:140:MET:O	2:K:144:ILE:HG13	2.17	0.43
2:L:155:SER:HB2	2:L:157:GLU:OE2	2.18	0.43
2:H:208:VAL:O	2:H:212:GLU:HG3	2.18	0.43
1:G:44:LEU:HD23	1:G:44:LEU:H	1.83	0.43
1:G:247:ILE:HD12	1:G:257:ASP:HA	2.01	0.43
1:G:257:ASP:O	1:G:261:ILE:HG13	2.19	0.43
1:C:275:LEU:HD12	1:C:321:ASN:HB3	2.00	0.43
1:F:187:SER:HA	2:I:127:ARG:NH1	2.33	0.43
1:A:79:THR:OG1	1:A:242:ASP:HB2	2.18	0.43
1:B:288:LEU:HD23	1:B:288:LEU:HA	1.84	0.43
2:E:200:LEU:N	2:E:200:LEU:HD23	2.33	0.43
2:K:140:MET:HE2	2:K:140:MET:HB3	1.86	0.43
1:F:13:VAL:HG13	1:F:16:SER:OG	2.17	0.43
1:B:296:LYS:HB3	1:B:296:LYS:HE2	1.66	0.43
2:D:164:ILE:HD12	2:D:164:ILE:HA	1.96	0.43
1:J:157:GLN:HG2	1:J:157:GLN:H	1.55	0.43
2:L:200:LEU:CD2	2:L:222:SER:OG	2.60	0.43
1:C:41:PRO:HD2	1:C:69:ALA:HA	2.01	0.43
1:C:202:THR:HB	1:C:205:THR:HG21	2.00	0.43
1:F:80:PRO:HG3	1:F:340:ASP:HA	2.00	0.43
1:F:157:GLN:H	1:F:157:GLN:HG2	1.65	0.43
2:L:123:MET:HE1	2:L:163:PHE:HB2	1.99	0.43
1:F:267:LYS:HG3	1:F:297:GLU:HG2	2.01	0.43
1:G:279:THR:HG22	1:G:300:LYS:HD2	2.00	0.43
2:I:217:LEU:HD11	2:I:230:VAL:HG22	2.00	0.43
1:J:268:HIS:HB2	1:J:351:THR:HG23	2.01	0.43
1:C:82:VAL:O	1:C:86:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ALA:O	1:C:102:ASN:HB2	2.19	0.43
2:I:191:SER:HB2	2:I:212:GLU:OE2	2.19	0.43
2:L:196:ILE:HD13	2:L:205:ARG:HA	2.00	0.43
1:A:50:ARG:NH1	1:A:103:PRO:O	2.51	0.43
1:J:340:ASP:HB3	1:J:343:LEU:HB3	2.01	0.43
2:K:144:ILE:HG12	2:K:175:ILE:HG21	2.01	0.43
1:G:61:VAL:HG13	1:G:71:VAL:HG11	2.01	0.43
1:B:227:PHE:CE1	1:B:231:LYS:HG3	2.54	0.42
2:K:202:THR:OG1	2:K:203:ARG:N	2.52	0.42
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.86	0.42
1:F:46:GLY:O	1:F:96:MET:HA	2.19	0.42
1:B:281:VAL:O	1:B:323:GLY:HA2	2.19	0.42
2:L:191:SER:HB2	2:L:212:GLU:OE2	2.17	0.42
1:B:330:LEU:O	1:B:339:GLY:HA2	2.19	0.42
1:A:14:ALA:HA	1:A:18:LEU:HB3	2.02	0.42
1:A:80:PRO:HG3	1:A:339:GLY:O	2.18	0.42
1:B:22:LEU:HD13	1:B:26:VAL:HG23	2.02	0.42
1:J:110:LYS:HD3	1:J:111:PHE:H	1.83	0.42
2:H:135:GLU:N	2:H:135:GLU:OE1	2.52	0.42
1:B:44:LEU:HD21	1:B:86:THR:HG22	2.01	0.42
1:B:100:SER:C	1:B:102:ASN:H	2.23	0.42
1:C:80:PRO:HG3	1:C:339:GLY:O	2.19	0.42
1:A:287:ASN:O	1:A:290:PHE:HB3	2.19	0.42
1:G:138:LEU:CD2	1:G:139:PRO:HD2	2.50	0.42
1:G:332:PHE:CE2	1:G:347:MET:HG3	2.54	0.42
1:C:208:ASN:O	1:C:208:ASN:ND2	2.52	0.42
1:F:342:LEU:H	1:F:342:LEU:HD12	1.84	0.42
1:A:308:ASP:OD1	1:A:308:ASP:N	2.53	0.42
1:B:152:TYR:CE2	2:D:126:ARG:HB3	2.55	0.42
1:J:274:ARG:O	1:J:321:ASN:ND2	2.52	0.42
1:C:134:PRO:HD2	1:C:135:GLU:OE2	2.20	0.42
1:A:280:VAL:HG13	1:A:322:VAL:HG12	2.01	0.42
1:C:13:VAL:HA	1:C:106:ASP:HA	2.02	0.42
2:I:119:ALA:O	2:I:122:TYR:HB3	2.20	0.42
2:I:201:GLY:O	2:I:203:ARG:N	2.53	0.42
1:A:3:LYS:HD2	1:A:3:LYS:HA	1.89	0.42
1:A:296:LYS:HE2	1:A:296:LYS:HB3	1.88	0.42
1:B:39:GLN:H	1:B:39:GLN:CD	2.23	0.42
1:B:100:SER:O	1:B:101:HIS:CG	2.73	0.42
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.89	0.42
1:G:28:ARG:NH1	1:G:67:ILE:HG23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ASN:OD1	1:G:150:ASN:N	2.53	0.42
2:K:107:GLU:HB3	2:K:108:ALA:H	1.65	0.42
1:F:296:LYS:HB3	1:F:296:LYS:HE2	1.73	0.42
1:A:175:HIS:HD2	1:A:199:ASP:O	2.02	0.41
2:K:127:ARG:NH2	2:K:224:GLU:HA	2.29	0.41
1:A:150:ASN:OD1	1:A:150:ASN:N	2.53	0.41
1:F:22:LEU:O	1:F:26:VAL:HG23	2.19	0.41
1:F:110:LYS:HD3	1:F:111:PHE:H	1.85	0.41
2:D:129:GLY:HA3	2:D:203:ARG:NH1	2.35	0.41
2:E:200:LEU:HD12	2:E:204:HIS:CG	2.55	0.41
1:G:335:TYR:HB2	1:G:343:LEU:HD21	2.03	0.41
2:L:200:LEU:HG	2:L:204:HIS:HD2	1.84	0.41
2:H:208:VAL:HG23	2:H:234:GLY:HA2	2.01	0.41
1:J:61:VAL:HA	1:J:64:LEU:HD12	2.02	0.41
2:D:203:ARG:H	2:D:203:ARG:HG2	1.69	0.41
1:J:245:ARG:HD3	1:J:327:SER:O	2.20	0.41
1:A:181:ALA:HA	1:A:216:VAL:HG23	2.02	0.41
1:B:157:GLN:HA	1:B:160:LEU:CB	2.47	0.41
2:E:214:THR:C	2:E:216:SER:H	2.23	0.41
1:G:185:THR:HG22	1:G:342:LEU:HD11	2.02	0.41
1:J:15:ASN:O	1:J:19:THR:HG22	2.21	0.41
2:K:164:ILE:HA	2:K:165:PRO:HD2	1.76	0.41
1:F:192:LEU:HD21	1:F:346:ILE:HD11	2.02	0.41
2:I:140:MET:HE3	2:I:143:TYR:CD2	2.55	0.41
1:A:50:ARG:HD3	1:A:106:ASP:O	2.21	0.41
1:A:244:ASP:OD1	1:A:245:ARG:HG3	2.21	0.41
2:K:112:THR:O	2:K:116:ILE:HG13	2.21	0.41
1:B:100:SER:O	1:B:102:ASN:N	2.53	0.41
2:D:112:THR:O	2:D:116:ILE:HG13	2.21	0.41
1:J:80:PRO:HG3	1:J:339:GLY:O	2.21	0.41
1:J:292:LYS:HD3	1:J:292:LYS:HA	1.86	0.41
2:K:122:TYR:O	2:K:126:ARG:HG3	2.20	0.41
2:L:143:TYR:CE1	2:L:189:PRO:HD3	2.56	0.41
1:F:26:VAL:HG22	1:F:131:MET:HE1	2.03	0.41
1:F:29:PHE:HD2	1:F:131:MET:HG2	1.85	0.41
2:I:116:ILE:HD11	2:I:176:MET:HE1	2.03	0.41
1:B:251:GLU:OE1	1:B:251:GLU:N	2.41	0.41
1:J:181:ALA:HA	1:J:216:VAL:HG23	2.02	0.41
2:K:164:ILE:O	2:K:166:ASN:N	2.54	0.41
1:C:140:ARG:HD3	1:F:15:ASN:OD1	2.20	0.41
1:F:104:VAL:HG21	1:F:210:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.93	0.41
2:K:123:MET:O	2:K:127:ARG:N	2.54	0.41
2:H:107:GLU:HB3	2:H:108:ALA:H	1.64	0.40
2:H:143:TYR:CE1	2:H:189:PRO:HD3	2.55	0.40
1:A:263:TYR:HE2	1:A:365:GLU:HB2	1.86	0.40
1:B:123:GLN:O	1:B:127:ILE:HG13	2.21	0.40
1:B:125:ALA:O	1:B:129:ARG:HG3	2.21	0.40
1:G:164:LYS:HG2	1:G:196:LEU:HD21	2.03	0.40
1:G:315:MET:HA	1:G:320:TYR:HB2	2.03	0.40
1:B:42:LYS:O	1:B:91:ALA:HB1	2.20	0.40
1:B:52:SER:O	1:B:56:LEU:HG	2.22	0.40
1:B:272:GLU:CD	1:B:274:ARG:HH11	2.24	0.40
1:G:115:ASP:N	1:G:115:ASP:OD1	2.54	0.40
1:F:146:LEU:HG	1:F:147:GLY:H	1.87	0.40
1:B:292:LYS:HA	1:B:292:LYS:HD3	1.81	0.40
1:G:52:SER:HA	1:J:146:LEU:CD2	2.51	0.40
1:A:78:SER:HB2	1:A:80:PRO:HD2	2.04	0.40
2:D:201:GLY:O	2:D:202:THR:OG1	2.36	0.40
2:E:201:GLY:C	2:E:202:THR:HG1	2.22	0.40
1:G:20:PRO:HA	1:G:23:ALA:HB3	2.02	0.40
1:C:54:HIS:CG	1:F:149:VAL:HG11	2.57	0.40
1:F:100:SER:O	1:F:101:HIS:CG	2.75	0.40
1:A:185:THR:HG22	1:A:342:LEU:HD21	2.03	0.40
1:G:366:MET:HG2	1:G:367:GLN:N	2.35	0.40
1:J:315:MET:HB3	1:J:333:LEU:HD12	2.04	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	367/369 (100%)	342 (93%)	22 (6%)	3 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	367/369 (100%)	347 (95%)	17 (5%)	3 (1%)	19	60
1	C	367/369 (100%)	339 (92%)	25 (7%)	3 (1%)	19	60
1	F	367/369 (100%)	343 (94%)	22 (6%)	2 (0%)	29	68
1	G	367/369 (100%)	340 (93%)	24 (6%)	3 (1%)	19	60
1	J	367/369 (100%)	344 (94%)	21 (6%)	2 (0%)	29	68
2	D	144/167 (86%)	128 (89%)	14 (10%)	2 (1%)	11	47
2	E	144/167 (86%)	122 (85%)	18 (12%)	4 (3%)	5	33
2	H	144/167 (86%)	128 (89%)	14 (10%)	2 (1%)	11	47
2	I	144/167 (86%)	129 (90%)	13 (9%)	2 (1%)	11	47
2	K	144/167 (86%)	126 (88%)	13 (9%)	5 (4%)	3	29
2	L	144/167 (86%)	127 (88%)	14 (10%)	3 (2%)	7	39
All	All	3066/3216 (95%)	2815 (92%)	217 (7%)	34 (1%)	14	52

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	100	SER
1	A	100	SER
1	B	100	SER
2	K	165	PRO
2	L	202	THR
1	C	37	ASP
2	H	202	THR
2	I	202	THR
2	D	202	THR
2	E	171	ASP
2	E	202	THR
1	G	37	ASP
1	J	100	SER
2	K	202	THR
1	C	100	SER
1	C	186	SER
1	F	101	HIS
2	H	165	PRO
2	I	165	PRO
1	B	37	ASP
1	B	101	HIS
2	E	239	GLU

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Mol	Chain	Res	Type
1	G	100	SER
2	K	112	THR
2	L	165	PRO
1	A	186	SER
2	K	171	ASP
1	A	37	ASP
2	D	199	GLU
1	G	101	HIS
1	J	101	HIS
2	E	162	ILE
2	K	239	GLU
2	L	199	GLU

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	294/294 (100%)	290 (99%)	4 (1%)	67	80
1	B	294/294 (100%)	291 (99%)	3 (1%)	76	86
1	C	294/294 (100%)	291 (99%)	3 (1%)	76	86
1	F	294/294 (100%)	292 (99%)	2 (1%)	84	90
1	G	294/294 (100%)	289 (98%)	5 (2%)	60	78
1	J	294/294 (100%)	292 (99%)	2 (1%)	84	90
2	D	120/139 (86%)	116 (97%)	4 (3%)	38	61
2	E	120/139 (86%)	117 (98%)	3 (2%)	47	68
2	H	120/139 (86%)	118 (98%)	2 (2%)	60	78
2	I	120/139 (86%)	117 (98%)	3 (2%)	47	68
2	K	120/139 (86%)	115 (96%)	5 (4%)	30	55
2	L	120/139 (86%)	117 (98%)	3 (2%)	47	68
All	All	2484/2598 (96%)	2445 (98%)	39 (2%)	62	79

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ASN
1	C	170	ASP
1	C	288	LEU
1	F	44	LEU
1	F	288	LEU
2	H	187	TYR
2	H	198	LYS
2	I	110	GLN
2	I	156	SER
2	I	232	LYS
1	A	90	ASP
1	A	244	ASP
1	A	288	LEU
1	A	366	MET
1	B	44	LEU
1	B	152	TYR
1	B	288	LEU
2	D	110	GLN
2	D	187	TYR
2	D	203	ARG
2	D	223	GLU
2	E	110	GLN
2	E	123	MET
2	E	187	TYR
1	G	187	SER
1	G	244	ASP
1	G	288	LEU
1	G	301	SER
1	G	366	MET
1	J	44	LEU
1	J	301	SER
2	K	110	GLN
2	K	178	ASN
2	K	187	TYR
2	K	203	ARG
2	K	222	SER
2	L	110	GLN
2	L	123	MET
2	L	187	TYR

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

Mol	Chain	Res	Type
1	C	213	ASN
1	F	213	ASN
1	G	213	ASN
2	K	204	HIS

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	368/369 (99%)	0.18	10 (2%) 54 44	77, 119, 150, 176	0
1	B	368/369 (99%)	0.50	18 (4%) 29 25	97, 135, 174, 192	0
1	C	368/369 (99%)	0.26	7 (1%) 66 58	77, 113, 149, 169	0
1	F	368/369 (99%)	0.16	5 (1%) 75 65	70, 102, 134, 158	0
1	G	368/369 (99%)	0.21	7 (1%) 66 58	83, 129, 156, 176	0
1	J	368/369 (99%)	0.29	2 (0%) 91 86	71, 118, 145, 164	0
2	D	146/167 (87%)	0.01	1 (0%) 87 82	76, 100, 140, 173	27 (18%)
2	E	146/167 (87%)	-0.06	0 100 100	71, 104, 119, 150	27 (18%)
2	H	146/167 (87%)	0.13	3 (2%) 63 54	72, 104, 137, 174	27 (18%)
2	I	146/167 (87%)	0.20	3 (2%) 63 54	77, 107, 129, 145	27 (18%)
2	K	146/167 (87%)	-0.01	0 100 100	68, 94, 115, 137	27 (18%)
2	L	146/167 (87%)	0.01	0 100 100	62, 96, 132, 155	27 (18%)
All	All	3084/3216 (95%)	0.20	56 (1%) 68 59	62, 113, 153, 192	162 (5%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLY	4.4
1	A	324	GLY	4.2
2	H	133	THR	3.9
1	G	2	GLY	3.5
1	J	324	GLY	3.3
1	C	93	ALA	3.0
1	C	112	PHE	2.9
1	G	335	TYR	2.8
1	B	56	LEU	2.8
1	G	349	MET	2.8
1	B	70	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	323	GLY	2.6
1	B	321	ASN	2.5
1	B	281	VAL	2.5
1	B	55	MET	2.4
1	B	92	GLU	2.4
1	C	111	PHE	2.4
1	F	94	GLY	2.4
1	B	5	PHE	2.4
1	B	2	GLY	2.3
2	I	133	THR	2.3
1	J	110	LYS	2.3
1	A	45	ILE	2.3
1	C	338	THR	2.3
1	C	92	GLU	2.3
1	F	303	GLN	2.3
1	C	309	ARG	2.3
1	F	95	VAL	2.3
1	B	224	LEU	2.3
1	B	280	VAL	2.3
1	F	2	GLY	2.2
2	H	218	THR	2.2
1	A	44	LEU	2.2
1	G	146	LEU	2.2
1	B	336	ASN	2.2
1	B	345	ALA	2.2
1	B	42	LYS	2.2
1	B	123	GLN	2.2
1	A	93	ALA	2.2
1	B	57	GLU	2.2
1	A	95	VAL	2.2
1	A	322	VAL	2.2
1	G	41	PRO	2.1
1	B	343	LEU	2.1
1	G	332	PHE	2.1
1	B	369	PHE	2.1
1	F	110	LYS	2.1
2	H	176	MET	2.1
1	B	112	PHE	2.1
2	I	249	LEU	2.0
1	G	164	LYS	2.0
2	I	132	LEU	2.0
2	D	188	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	124	GLU	2.0
1	A	110	LYS	2.0
1	A	241	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.