Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:40 AM UTC

PDB ID	:	7OLH / pdb_00007olh
Title	:	Bacillus subtilis Complex structure 1 of diadenylate cyclase CdaA cytoplasmic domain (CdaACD) and the phosphoglucomutase GlmM short variant (GlmMF369)
Authors	:	Pathania, M.; Grundling, A.G.; Freemont, P.
Deposited on	:	2021-05-20
Resolution	:	3.65 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

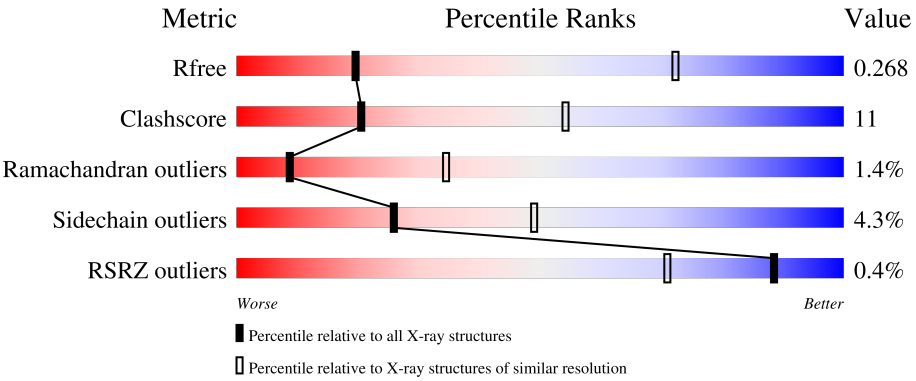
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	464	57% 21% 21%
1	B	464	60% 19% 21%
1	C	464	59% 19% 21%
1	D	464	60% 19% 21%
1	E	464	61% 18% 21%

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Mol	Chain	Length	Quality of chain
1	F	464	61% 18% 21%
2	G	167	60% 22% 6% 13%
2	H	167	62% 18% 7% 14%
2	I	167	56% 28% 13%
2	J	167	53% 29% 6% 12%
2	K	167	60% 23% 13%
2	L	167	64% 19% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23157 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	A	368	Total	C	N	O	S	0	1	0
			2762	1731	464	553	14			
1	B	366	Total	C	N	O	S	0	1	0
			2747	1720	462	551	14			
1	C	368	Total	C	N	O	S	0	1	0
			2762	1731	464	553	14			
1	D	367	Total	C	N	O	S	0	1	0
			2758	1729	463	552	14			
1	E	367	Total	C	N	O	S	0	1	0
			2758	1729	463	552	14			
1	F	367	Total	C	N	O	S	0	1	0
			2751	1722	463	552	14			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	LEU	-	expression tag	UNP O34824
A	450	VAL	-	expression tag	UNP O34824
A	451	PRO	-	expression tag	UNP O34824
A	452	ARG	-	expression tag	UNP O34824
A	453	GLY	-	expression tag	UNP O34824
A	454	SER	-	expression tag	UNP O34824
A	455	SER	-	expression tag	UNP O34824
A	456	GLY	-	expression tag	UNP O34824
A	457	LEU	-	expression tag	UNP O34824
A	458	GLU	-	expression tag	UNP O34824
A	459	HIS	-	expression tag	UNP O34824
A	460	HIS	-	expression tag	UNP O34824
A	461	HIS	-	expression tag	UNP O34824
A	462	HIS	-	expression tag	UNP O34824
A	463	HIS	-	expression tag	UNP O34824
A	464	HIS	-	expression tag	UNP O34824
B	449	LEU	-	expression tag	UNP O34824

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Chain	Residue	Modelled	Actual	Comment	Reference
B	450	VAL	-	expression tag	UNP O34824
B	451	PRO	-	expression tag	UNP O34824
B	452	ARG	-	expression tag	UNP O34824
B	453	GLY	-	expression tag	UNP O34824
B	454	SER	-	expression tag	UNP O34824
B	455	SER	-	expression tag	UNP O34824
B	456	GLY	-	expression tag	UNP O34824
B	457	LEU	-	expression tag	UNP O34824
B	458	GLU	-	expression tag	UNP O34824
B	459	HIS	-	expression tag	UNP O34824
B	460	HIS	-	expression tag	UNP O34824
B	461	HIS	-	expression tag	UNP O34824
B	462	HIS	-	expression tag	UNP O34824
B	463	HIS	-	expression tag	UNP O34824
B	464	HIS	-	expression tag	UNP O34824
C	449	LEU	-	expression tag	UNP O34824
C	450	VAL	-	expression tag	UNP O34824
C	451	PRO	-	expression tag	UNP O34824
C	452	ARG	-	expression tag	UNP O34824
C	453	GLY	-	expression tag	UNP O34824
C	454	SER	-	expression tag	UNP O34824
C	455	SER	-	expression tag	UNP O34824
C	456	GLY	-	expression tag	UNP O34824
C	457	LEU	-	expression tag	UNP O34824
C	458	GLU	-	expression tag	UNP O34824
C	459	HIS	-	expression tag	UNP O34824
C	460	HIS	-	expression tag	UNP O34824
C	461	HIS	-	expression tag	UNP O34824
C	462	HIS	-	expression tag	UNP O34824
C	463	HIS	-	expression tag	UNP O34824
C	464	HIS	-	expression tag	UNP O34824
D	449	LEU	-	expression tag	UNP O34824
D	450	VAL	-	expression tag	UNP O34824
D	451	PRO	-	expression tag	UNP O34824
D	452	ARG	-	expression tag	UNP O34824
D	453	GLY	-	expression tag	UNP O34824
D	454	SER	-	expression tag	UNP O34824
D	455	SER	-	expression tag	UNP O34824
D	456	GLY	-	expression tag	UNP O34824
D	457	LEU	-	expression tag	UNP O34824
D	458	GLU	-	expression tag	UNP O34824
D	459	HIS	-	expression tag	UNP O34824

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Chain	Residue	Modelled	Actual	Comment	Reference
D	460	HIS	-	expression tag	UNP O34824
D	461	HIS	-	expression tag	UNP O34824
D	462	HIS	-	expression tag	UNP O34824
D	463	HIS	-	expression tag	UNP O34824
D	464	HIS	-	expression tag	UNP O34824
E	449	LEU	-	expression tag	UNP O34824
E	450	VAL	-	expression tag	UNP O34824
E	451	PRO	-	expression tag	UNP O34824
E	452	ARG	-	expression tag	UNP O34824
E	453	GLY	-	expression tag	UNP O34824
E	454	SER	-	expression tag	UNP O34824
E	455	SER	-	expression tag	UNP O34824
E	456	GLY	-	expression tag	UNP O34824
E	457	LEU	-	expression tag	UNP O34824
E	458	GLU	-	expression tag	UNP O34824
E	459	HIS	-	expression tag	UNP O34824
E	460	HIS	-	expression tag	UNP O34824
E	461	HIS	-	expression tag	UNP O34824
E	462	HIS	-	expression tag	UNP O34824
E	463	HIS	-	expression tag	UNP O34824
E	464	HIS	-	expression tag	UNP O34824
F	449	LEU	-	expression tag	UNP O34824
F	450	VAL	-	expression tag	UNP O34824
F	451	PRO	-	expression tag	UNP O34824
F	452	ARG	-	expression tag	UNP O34824
F	453	GLY	-	expression tag	UNP O34824
F	454	SER	-	expression tag	UNP O34824
F	455	SER	-	expression tag	UNP O34824
F	456	GLY	-	expression tag	UNP O34824
F	457	LEU	-	expression tag	UNP O34824
F	458	GLU	-	expression tag	UNP O34824
F	459	HIS	-	expression tag	UNP O34824
F	460	HIS	-	expression tag	UNP O34824
F	461	HIS	-	expression tag	UNP O34824
F	462	HIS	-	expression tag	UNP O34824
F	463	HIS	-	expression tag	UNP O34824
F	464	HIS	-	expression tag	UNP O34824

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			

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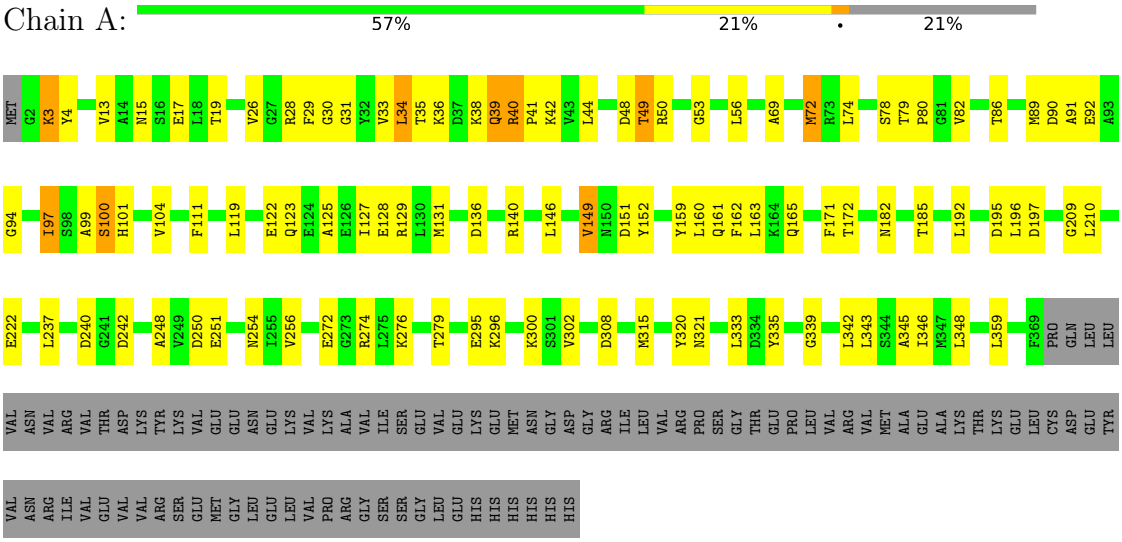
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	144	Total	C	N	O	S	103	0	0
			1092	683	185	219	5			
2	I	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	J	147	Total	C	N	O	S	103	0	0
			1117	701	188	223	5			
2	K	146	Total	C	N	O	S	121	0	0
			1106	692	187	222	5			
2	L	144	Total	C	N	O	S	103	0	0
			1092	683	185	219	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.

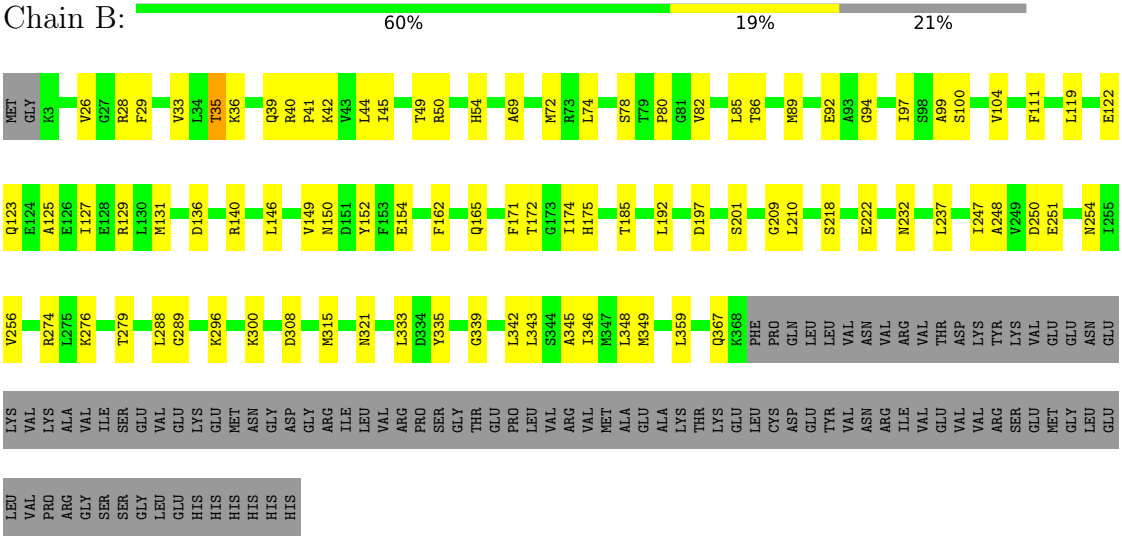
• Molecule 1: Phosphoglucosamine mutase

Chain A:



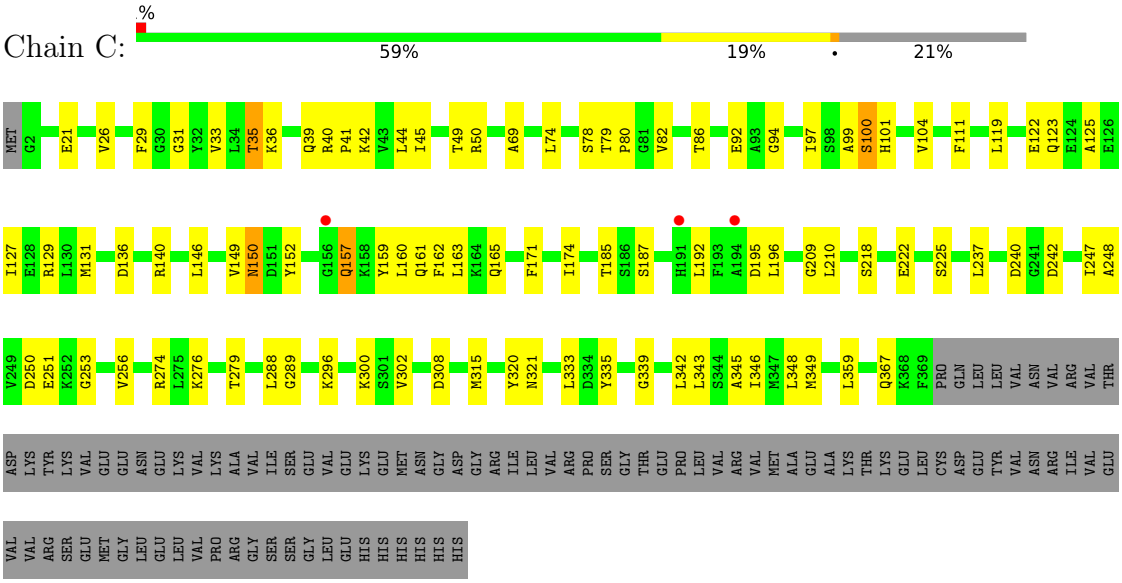
• Molecule 1: Phosphoglucosamine mutase

Chain B:



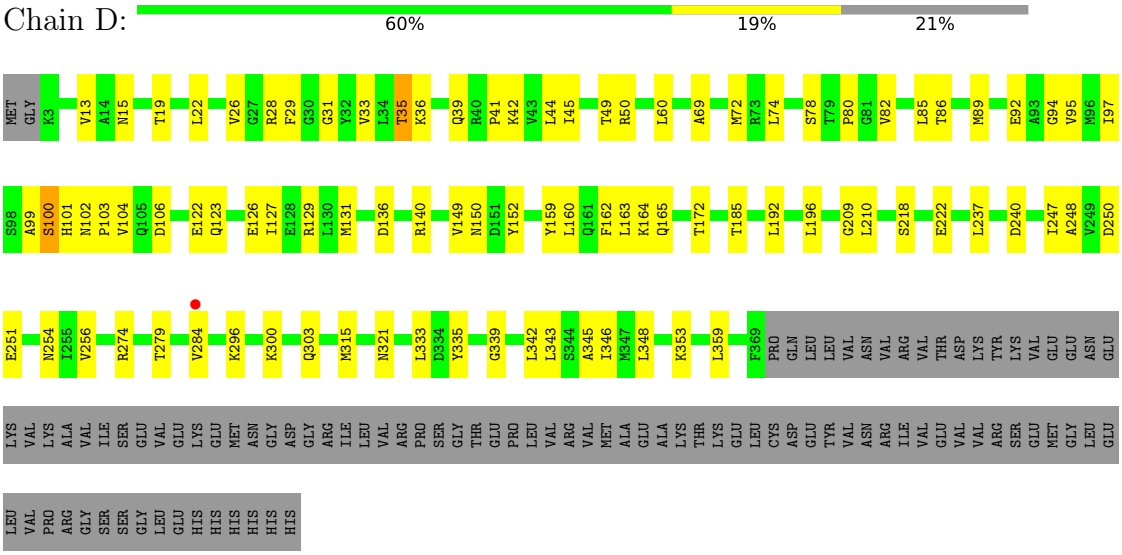
• Molecule 1: Phosphoglucosamine mutase

Chain C:



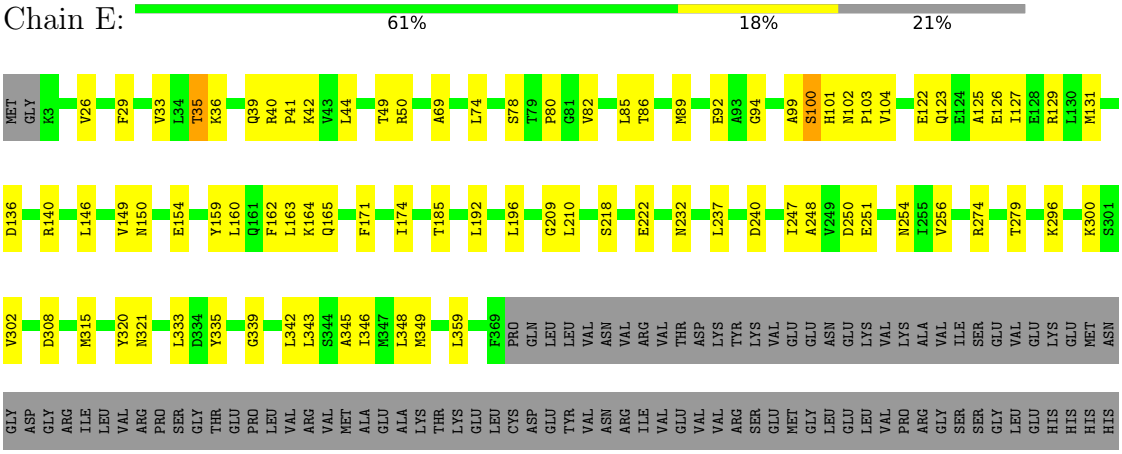
• Molecule 1: Phosphoglucosamine mutase

Chain D:



• Molecule 1: Phosphoglucosamine mutase

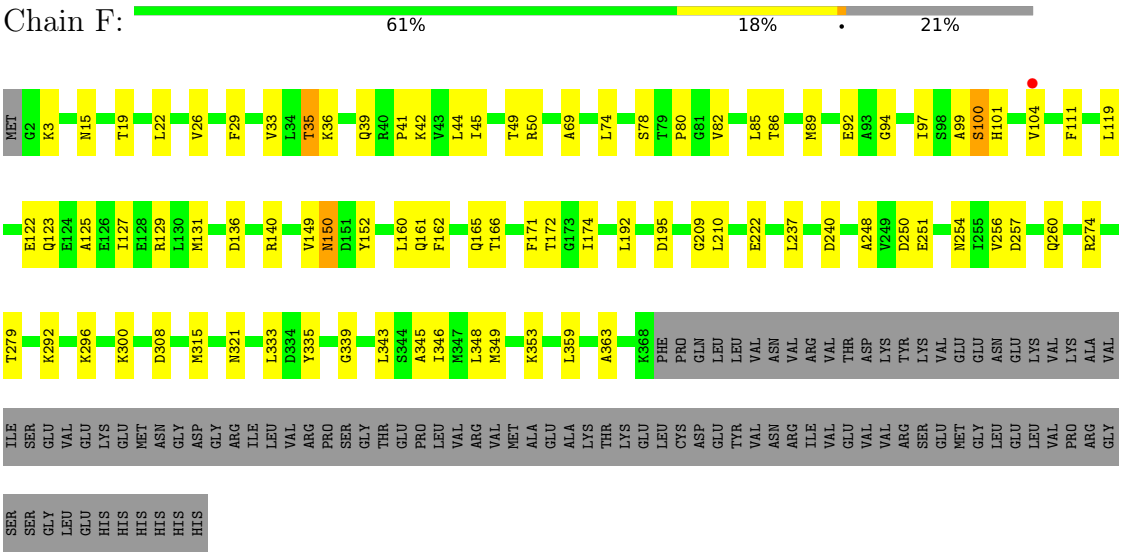
Chain E:





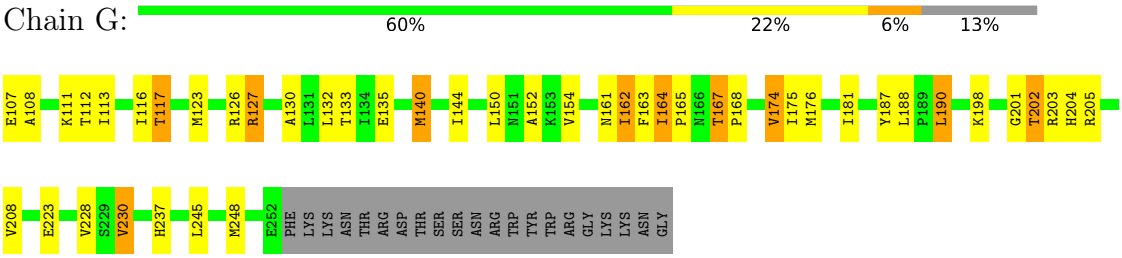
• Molecule 1: Phosphoglucosamine mutase

Chain F:



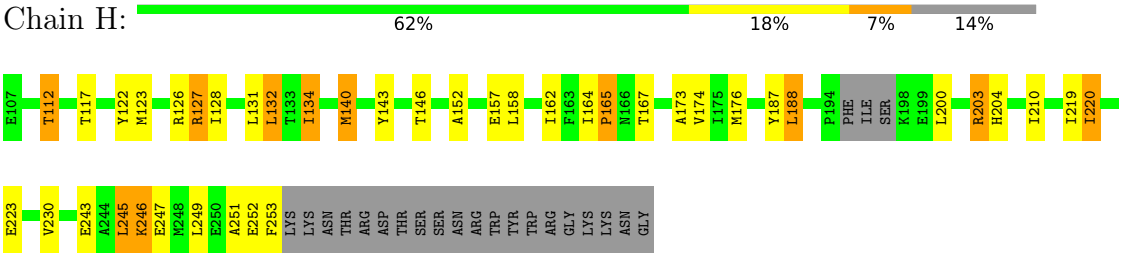
• Molecule 2: Cyclic di-AMP synthase CdaA

Chain G:



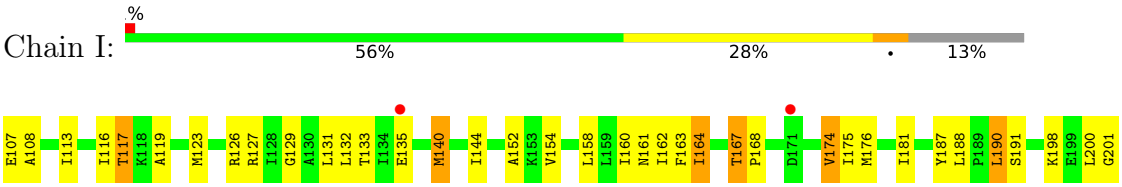
• Molecule 2: Cyclic di-AMP synthase CdaA

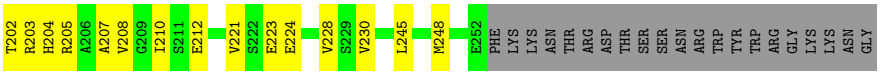
Chain H:



• Molecule 2: Cyclic di-AMP synthase CdaA

Chain I:



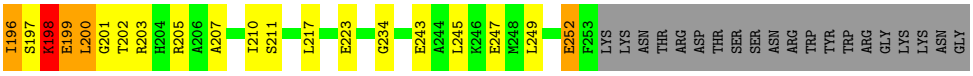


• Molecule 2: Cyclic di-AMP synthase CdaA

Chain J:



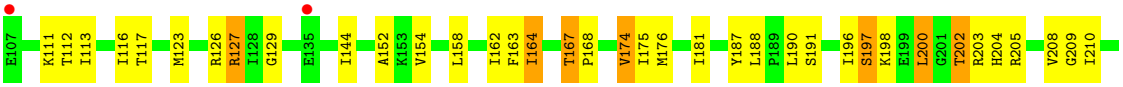


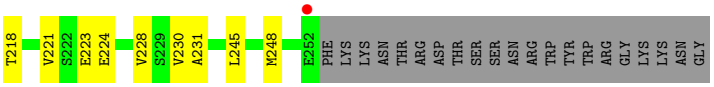


• Molecule 2: Cyclic di-AMP synthase CdaA

Chain K:



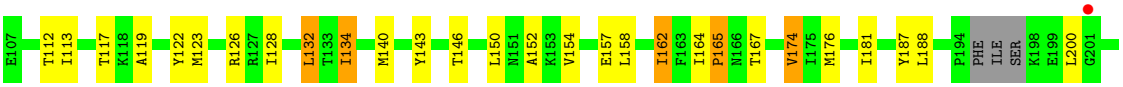


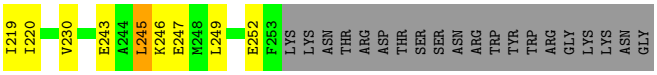


• Molecule 2: Cyclic di-AMP synthase CdaA

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	62.20Å 227.56Å 151.60Å 90.00° 99.66° 90.00°	Depositor
Resolution (Å)	61.32 – 3.65 61.32 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (61.32-3.65) 99.4 (61.32-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.242 , 0.262 0.247 , 0.268	Depositor DCC
R_{free} test set	2177 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	109.3	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23157	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.14	0/2806	0.38	0/3781
1	B	0.13	0/2790	0.34	0/3760
1	C	0.13	0/2806	0.34	0/3781
1	D	0.12	0/2802	0.33	0/3776
1	E	0.12	0/2802	0.33	0/3776
1	F	0.12	0/2794	0.33	0/3765
2	G	0.17	0/1118	0.49	0/1512
2	H	0.17	0/1103	0.49	0/1490
2	I	0.18	0/1118	0.49	0/1512
2	J	0.20	0/1130	0.53	0/1528
2	K	0.20	0/1118	0.48	0/1512
2	L	0.17	0/1103	0.49	0/1490
All	All	0.15	0/23490	0.39	0/31683

There are no bond length outliers.

There are no bond angle outliers.

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	71	0
1	B	2747	0	2720	56	0
1	C	2762	0	2732	60	0
1	D	2758	0	2729	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2758	0	2729	52	0
1	F	2751	0	2723	56	0
2	G	1106	0	1128	38	0
2	H	1092	0	1111	31	0
2	I	1106	0	1128	36	0
2	J	1117	0	1137	27	0
2	K	1106	0	1128	30	0
2	L	1092	0	1111	25	0
All	All	23157	0	23108	502	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 11.

All (502) 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:K:123:MET:HE1	2:K:163:PHE:HB2	1.33	1.06
2:I:123:MET:HE1	2:I:163:PHE:HB2	1.49	0.92
1:C:157:GLN:HE22	2:G:165:PRO:HD2	1.50	0.75
1:A:192:LEU:HD21	1:A:346:ILE:HD11	1.69	0.74
1:B:154:GLU:HG2	2:I:187:TYR:CZ	2.24	0.73
1:A:89:MET:HE2	2:J:127:ARG:HB2	1.70	0.73
2:J:164:ILE:O	2:J:167:THR:OG1	2.07	0.73
2:K:154:VAL:HG21	2:K:176:MET:HE3	1.73	0.71
1:E:50:ARG:NH2	1:E:99:ALA:O	2.26	0.69
1:F:42:LYS:H	1:F:92:GLU:HG2	1.58	0.69
1:D:42:LYS:H	1:D:92:GLU:HG2	1.58	0.69
1:F:192:LEU:HD21	1:F:346:ILE:HD11	1.74	0.69
2:K:127:ARG:NH2	2:K:223:GLU:O	2.26	0.69
1:E:44:LEU:HD12	1:E:74:LEU:HD11	1.75	0.68
2:K:197:SER:HB2	2:K:200:LEU:HD21	1.75	0.68
1:B:85:LEU:HB3	1:B:89:MET:HE3	1.76	0.68
1:A:86:THR:HG21	1:A:94:GLY:HA3	1.75	0.68
2:I:154:VAL:HG21	2:I:176:MET:HE3	1.76	0.68
2:L:113:ILE:O	2:L:117:THR:HG23	1.94	0.67
1:E:42:LYS:H	1:E:92:GLU:HG2	1.59	0.67
1:E:85:LEU:HB3	1:E:89:MET:HE3	1.76	0.67
1:A:97:ILE:O	1:A:97:ILE:HG13	1.94	0.67
2:G:154:VAL:HG21	2:G:176:MET:HE3	1.77	0.67
2:L:117:THR:HG21	2:L:246:LYS:HE3	1.77	0.66
1:D:50:ARG:NH2	1:D:99:ALA:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:127:ARG:NH2	2:I:223:GLU:O	2.29	0.66
1:A:26:VAL:HG22	1:A:131:MET:HE1	1.76	0.66
1:B:42:LYS:H	1:B:92:GLU:HG2	1.61	0.66
2:H:122:TYR:O	2:H:126:ARG:HG2	1.95	0.66
1:C:35:THR:HA	1:C:41:PRO:HG3	1.78	0.66
1:C:192:LEU:HD21	1:C:346:ILE:HD11	1.78	0.65
1:C:42:LYS:H	1:C:92:GLU:HG2	1.61	0.65
2:G:127:ARG:NH2	2:G:223:GLU:O	2.29	0.65
2:H:123:MET:HB3	2:H:128:ILE:HB	1.78	0.65
1:A:42:LYS:H	1:A:92:GLU:HG2	1.61	0.65
1:C:274:ARG:O	1:C:321:ASN:ND2	2.30	0.65
2:J:154:VAL:HG13	2:J:155:SER:H	1.62	0.65
1:F:44:LEU:HD12	1:F:74:LEU:HD11	1.79	0.64
1:A:40:ARG:NH2	1:A:146:LEU:O	2.31	0.64
1:A:151:ASP:O	2:J:126:ARG:NH2	2.31	0.64
1:C:44:LEU:HD12	1:C:74:LEU:HD11	1.79	0.64
2:G:113:ILE:O	2:G:117:THR:HG23	1.98	0.64
2:L:122:TYR:O	2:L:126:ARG:HG2	1.98	0.64
1:C:50:ARG:NH2	1:C:99:ALA:O	2.31	0.63
1:D:192:LEU:HD21	1:D:346:ILE:HD11	1.80	0.63
1:E:26:VAL:HG22	1:E:131:MET:HE1	1.79	0.63
1:A:162:PHE:O	1:A:165:GLN:HG3	1.99	0.63
1:B:136:ASP:OD2	1:B:140:ARG:NH2	2.31	0.63
1:E:41:PRO:HD2	1:E:69:ALA:HA	1.81	0.63
1:A:31:GLY:O	1:A:35:THR:OG1	2.13	0.62
1:B:41:PRO:HD2	1:B:69:ALA:HA	1.80	0.62
1:B:335:TYR:HB2	1:B:343:LEU:HD21	1.81	0.62
2:H:245:LEU:O	2:H:247:GLU:N	2.32	0.62
1:D:86:THR:HG21	1:D:94:GLY:HA3	1.82	0.62
1:E:192:LEU:HD21	1:E:346:ILE:HD11	1.81	0.62
2:I:123:MET:CE	2:I:163:PHE:HB2	2.27	0.62
1:A:274:ARG:O	1:A:321:ASN:ND2	2.33	0.62
1:C:136:ASP:OD2	1:C:140:ARG:NH2	2.32	0.61
1:C:195:ASP:OD1	2:G:126:ARG:NH1	2.33	0.61
1:D:26:VAL:HG22	1:D:131:MET:HE1	1.82	0.61
1:F:335:TYR:HB2	1:F:343:LEU:HD21	1.81	0.61
1:C:86:THR:HG21	1:C:94:GLY:HA3	1.81	0.61
1:F:26:VAL:HG22	1:F:131:MET:HE1	1.82	0.61
1:D:44:LEU:HD12	1:D:74:LEU:HD11	1.83	0.61
1:D:335:TYR:HB2	1:D:343:LEU:HD21	1.82	0.61
1:A:44:LEU:HD12	1:A:74:LEU:HD11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:VAL:HG22	1:C:131:MET:HE1	1.83	0.60
1:A:53:GLY:HA2	1:A:97:ILE:HD11	1.82	0.60
1:F:35:THR:HA	1:F:41:PRO:HG3	1.83	0.60
2:I:113:ILE:O	2:I:117:THR:HG23	2.01	0.60
1:B:162:PHE:O	1:B:165:GLN:HG3	2.01	0.60
1:E:136:ASP:OD2	1:E:140:ARG:NH2	2.33	0.60
1:E:162:PHE:O	1:E:165:GLN:HG3	2.01	0.60
2:H:203:ARG:HB3	2:H:220:ILE:HD13	1.83	0.60
2:L:123:MET:HB3	2:L:128:ILE:HB	1.82	0.60
1:E:35:THR:HA	1:E:41:PRO:HG3	1.84	0.60
1:F:86:THR:HG21	1:F:94:GLY:HA3	1.82	0.60
1:D:41:PRO:HD2	1:D:69:ALA:HA	1.83	0.60
1:F:195:ASP:OD1	2:K:126:ARG:NH1	2.35	0.60
2:G:150:LEU:HD22	2:H:158:LEU:HD22	1.84	0.60
1:E:335:TYR:HB2	1:E:343:LEU:HD21	1.84	0.60
1:B:49:THR:O	1:B:209:GLY:HA2	2.02	0.59
1:A:295:GLU:HB3	1:C:288:LEU:HD21	1.85	0.59
1:D:35:THR:HA	1:D:41:PRO:HG3	1.84	0.59
1:D:49:THR:O	1:D:209:GLY:HA2	2.02	0.59
2:K:144:ILE:HG12	2:K:175:ILE:HG21	1.84	0.59
1:B:35:THR:HA	1:B:41:PRO:HG3	1.84	0.59
1:E:49:THR:O	1:E:209:GLY:HA2	2.02	0.59
1:B:279:THR:HG22	1:B:300:LYS:HB2	1.84	0.59
1:F:49:THR:O	1:F:209:GLY:HA2	2.02	0.59
1:F:162:PHE:O	1:F:165:GLN:HG3	2.03	0.59
1:A:335:TYR:HB2	1:A:343:LEU:HD21	1.84	0.59
1:B:86:THR:HG21	1:B:94:GLY:HA3	1.83	0.58
1:D:100:SER:OG	1:D:240:ASP:OD2	2.20	0.58
1:E:104:VAL:HG21	1:E:210:LEU:HA	1.86	0.58
2:L:143:TYR:O	2:L:146:THR:HG22	2.04	0.58
2:I:158:LEU:HD22	2:J:150:LEU:HD22	1.86	0.58
1:E:40:ARG:NH2	1:E:146:LEU:O	2.37	0.58
1:A:39:GLN:O	1:A:40:ARG:HB2	2.03	0.58
1:B:192:LEU:HD21	1:B:346:ILE:HD11	1.85	0.58
2:K:158:LEU:HD22	2:L:150:LEU:HD22	1.86	0.57
1:A:3:LYS:HG3	1:A:4:TYR:CD1	2.39	0.57
1:C:40:ARG:NH2	1:C:146:LEU:O	2.37	0.57
1:C:41:PRO:HD2	1:C:69:ALA:HA	1.85	0.57
2:L:246:LYS:HA	2:L:249:LEU:HB2	1.86	0.57
1:B:50:ARG:NH2	1:B:99:ALA:O	2.38	0.57
1:D:315:MET:HE2	1:D:333:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:HD11	1:D:192:LEU:HB2	1.86	0.57
1:C:162:PHE:O	1:C:165:GLN:HG3	2.04	0.57
1:B:26:VAL:HG22	1:B:131:MET:HE1	1.86	0.57
2:I:123:MET:HE3	2:I:160:ILE:HA	1.86	0.56
1:C:335:TYR:HB2	1:C:343:LEU:HD21	1.87	0.56
1:D:44:LEU:HD21	1:D:86:THR:HG22	1.85	0.56
1:F:41:PRO:HD2	1:F:69:ALA:HA	1.87	0.56
1:B:248:ALA:HB3	1:B:256:VAL:HB	1.86	0.56
1:C:248:ALA:HB3	1:C:256:VAL:HB	1.86	0.56
1:E:86:THR:HG21	1:E:94:GLY:HA3	1.86	0.56
1:F:248:ALA:HB3	1:F:256:VAL:HB	1.88	0.56
2:H:219:ILE:HD11	2:H:249:LEU:HD21	1.88	0.56
2:G:123:MET:HE3	2:G:163:PHE:HB2	1.87	0.56
1:B:44:LEU:HD12	1:B:74:LEU:HD11	1.87	0.56
1:D:162:PHE:O	1:D:165:GLN:HG3	2.05	0.56
2:H:117:THR:HG21	2:H:246:LYS:HB2	1.87	0.56
1:E:44:LEU:HD21	1:E:86:THR:HG22	1.88	0.56
1:B:315:MET:HE2	1:B:333:LEU:HD12	1.87	0.55
2:H:143:TYR:O	2:H:146:THR:HG22	2.07	0.55
1:F:152:TYR:CE1	2:L:126:ARG:HB3	2.42	0.55
2:J:177:LYS:O	2:J:179:ASN:N	2.39	0.55
1:C:49:THR:O	1:C:209:GLY:HA2	2.06	0.55
2:G:144:ILE:HG12	2:G:175:ILE:HG21	1.89	0.55
2:L:245:LEU:HD22	2:L:246:LYS:H	1.72	0.55
1:A:80:PRO:HG3	1:A:339:GLY:O	2.07	0.55
2:I:154:VAL:HG22	2:I:181:ILE:HG13	1.88	0.55
1:A:44:LEU:HB3	1:A:72:MET:HB3	1.89	0.55
2:I:129:GLY:HA2	2:I:221:VAL:O	2.07	0.55
1:F:172:THR:O	1:F:353:LYS:NZ	2.39	0.55
2:J:158:LEU:O	2:J:162:ILE:HG13	2.07	0.55
1:A:111:PHE:HB3	1:A:119:LEU:HD13	1.88	0.54
1:C:225:SER:OG	1:C:253:GLY:O	2.22	0.54
2:I:158:LEU:O	2:I:162:ILE:HG12	2.08	0.54
2:I:204:HIS:O	2:I:208:VAL:HG12	2.08	0.54
1:A:44:LEU:HD21	1:A:86:THR:HG22	1.90	0.54
1:E:248:ALA:HB3	1:E:256:VAL:HB	1.89	0.54
1:A:279:THR:HG22	1:A:300:LYS:HB2	1.88	0.54
1:D:104:VAL:HG21	1:D:210:LEU:HA	1.88	0.54
1:D:251:GLU:OE1	1:D:251:GLU:N	2.38	0.54
1:F:82:VAL:O	1:F:86:THR:HG23	2.07	0.53
1:E:251:GLU:OE1	1:E:251:GLU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:HB3	1:A:256:VAL:HB	1.89	0.53
1:E:82:VAL:O	1:E:86:THR:HG23	2.08	0.53
2:K:202:THR:OG1	2:K:203:ARG:N	2.41	0.53
1:A:56:LEU:HB2	1:A:97:ILE:HD13	1.91	0.53
1:C:150:ASN:OD1	1:C:150:ASN:N	2.42	0.53
1:B:274:ARG:O	1:B:321:ASN:ND2	2.42	0.53
1:D:82:VAL:O	1:D:86:THR:HG23	2.09	0.53
1:E:126:GLU:OE2	1:E:129:ARG:NH1	2.41	0.53
2:J:211:SER:HB3	2:J:234:GLY:H	1.74	0.53
1:A:30:GLY:O	1:A:34:LEU:HG	2.09	0.53
2:G:135:GLU:HG3	2:G:140:MET:HG3	1.91	0.53
1:A:149:VAL:HG11	1:B:54:HIS:CG	2.44	0.53
1:D:80:PRO:HG3	1:D:339:GLY:O	2.09	0.53
2:I:119:ALA:O	2:I:123:MET:HG3	2.09	0.53
1:A:50:ARG:NH2	1:A:99:ALA:O	2.42	0.53
2:I:135:GLU:HG3	2:I:140:MET:HG3	1.89	0.53
2:K:113:ILE:O	2:K:117:THR:HG23	2.08	0.53
1:B:82:VAL:O	1:B:86:THR:HG23	2.08	0.52
1:F:136:ASP:OD2	1:F:140:ARG:NH2	2.42	0.52
1:C:171:PHE:HB3	1:C:174:ILE:HD12	1.91	0.52
1:A:251:GLU:N	1:A:251:GLU:OE1	2.40	0.52
1:C:276:LYS:H	1:C:321:ASN:HB2	1.74	0.52
1:E:174:ILE:HG21	1:E:349:MET:HE1	1.92	0.52
1:F:161:GLN:HG3	2:L:165:PRO:HB3	1.91	0.52
1:C:82:VAL:O	1:C:86:THR:HG23	2.09	0.52
1:D:72:MET:HE2	1:D:152:TYR:HB2	1.92	0.52
1:F:104:VAL:HG21	1:F:210:LEU:HA	1.91	0.52
1:F:251:GLU:OE1	1:F:251:GLU:N	2.41	0.52
2:K:228:VAL:HG11	2:K:245:LEU:HD22	1.92	0.52
1:B:175:HIS:NE2	1:B:201:SER:OG	2.41	0.52
1:C:251:GLU:OE1	1:C:251:GLU:N	2.40	0.52
2:G:111:LYS:O	2:G:112:THR:OG1	2.27	0.52
1:A:35:THR:HA	1:A:41:PRO:HG3	1.92	0.51
1:F:315:MET:HE2	1:F:333:LEU:HD12	1.92	0.51
1:E:250:ASP:OD1	1:E:254:ASN:N	2.43	0.51
1:B:80:PRO:HG3	1:B:339:GLY:O	2.11	0.51
1:A:82:VAL:O	1:A:86:THR:HG23	2.11	0.51
1:D:274:ARG:O	1:D:321:ASN:ND2	2.44	0.51
1:F:250:ASP:OD1	1:F:254:ASN:N	2.40	0.51
2:I:161:ASN:ND2	2:J:161:ASN:O	2.43	0.51
1:F:279:THR:HG22	1:F:300:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:O	1:A:49:THR:OG1	2.29	0.51
1:B:44:LEU:HD21	1:B:86:THR:HG22	1.93	0.51
1:E:29:PHE:HD2	1:E:131:MET:HG2	1.76	0.51
1:A:49:THR:O	1:A:209:GLY:HA2	2.11	0.50
1:A:136:ASP:OD2	1:A:140:ARG:NH2	2.39	0.50
1:B:251:GLU:OE1	1:B:251:GLU:N	2.43	0.50
1:D:78:SER:HB2	1:D:80:PRO:HD2	1.93	0.50
2:G:201:GLY:O	2:G:203:ARG:N	2.44	0.50
1:A:41:PRO:HD2	1:A:69:ALA:HA	1.93	0.50
1:E:100:SER:OG	1:E:240:ASP:OD2	2.29	0.50
1:E:164:LYS:HG2	1:E:196:LEU:HD21	1.93	0.50
1:F:44:LEU:HD21	1:F:86:THR:HG22	1.93	0.50
1:F:80:PRO:HG3	1:F:339:GLY:O	2.11	0.50
1:C:29:PHE:HD2	1:C:131:MET:HG2	1.77	0.50
1:B:29:PHE:HD2	1:B:131:MET:HG2	1.76	0.50
1:B:40:ARG:NH2	1:B:146:LEU:O	2.44	0.50
1:C:21:GLU:OE2	1:D:140:ARG:NH2	2.33	0.50
1:D:172:THR:O	1:D:353:LYS:NZ	2.42	0.50
1:D:348:LEU:HD21	1:D:359:LEU:HD13	1.92	0.50
1:E:279:THR:HG22	1:E:300:LYS:HB2	1.93	0.50
2:J:179:ASN:O	2:J:179:ASN:ND2	2.45	0.50
2:K:163:PHE:HZ	2:K:174:VAL:HB	1.77	0.50
1:C:44:LEU:HD21	1:C:86:THR:HG22	1.93	0.50
1:D:50:ARG:NH1	1:D:103:PRO:O	2.45	0.50
2:H:158:LEU:O	2:H:162:ILE:HG13	2.12	0.50
2:L:219:ILE:HD11	2:L:249:LEU:HD21	1.94	0.50
2:G:161:ASN:ND2	2:H:162:ILE:HA	2.27	0.50
2:I:228:VAL:HG11	2:I:245:LEU:HD22	1.93	0.50
1:F:50:ARG:NH2	1:F:99:ALA:O	2.44	0.50
1:F:160:LEU:HD11	1:F:192:LEU:HB2	1.94	0.50
1:D:248:ALA:HB3	1:D:256:VAL:HB	1.93	0.49
1:E:232:ASN:O	1:E:232:ASN:ND2	2.44	0.49
2:H:112:THR:HG23	2:H:176:MET:HE1	1.94	0.49
1:B:39:GLN:H	1:B:39:GLN:CD	2.20	0.49
1:B:171:PHE:HB3	1:B:174:ILE:HD12	1.94	0.49
1:A:160:LEU:HD11	1:A:192:LEU:HB2	1.94	0.49
1:C:111:PHE:HB3	1:C:119:LEU:HD13	1.93	0.49
1:A:78:SER:HB2	1:A:80:PRO:HD2	1.95	0.49
1:F:171:PHE:HB3	1:F:174:ILE:HD12	1.93	0.49
2:G:190:LEU:HD13	2:G:205:ARG:HB3	1.94	0.49
1:C:39:GLN:H	1:C:39:GLN:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:PRO:HG3	1:E:339:GLY:O	2.12	0.49
1:A:104:VAL:HG21	1:A:210:LEU:HA	1.95	0.49
1:F:78:SER:HB2	1:F:80:PRO:HD2	1.94	0.49
2:L:134:ILE:HA	2:L:176:MET:HB2	1.95	0.49
1:A:348:LEU:HD21	1:A:359:LEU:HD13	1.95	0.49
1:A:237:LEU:HD13	1:A:345:ALA:HB1	1.95	0.49
2:G:228:VAL:HG11	2:G:245:LEU:HD22	1.95	0.49
2:J:123:MET:HB3	2:J:128:ILE:HB	1.94	0.49
2:G:133:THR:HB	2:G:175:ILE:HD13	1.94	0.48
2:H:204:HIS:CD2	2:H:220:ILE:HG12	2.49	0.48
1:F:308:ASP:OD1	1:F:308:ASP:N	2.46	0.48
2:I:144:ILE:HG12	2:I:175:ILE:HG21	1.95	0.48
1:D:250:ASP:OD1	1:D:254:ASN:N	2.45	0.48
1:F:39:GLN:H	1:F:39:GLN:CD	2.21	0.48
1:F:348:LEU:HD21	1:F:359:LEU:HD13	1.95	0.48
1:C:237:LEU:HD13	1:C:345:ALA:HB1	1.96	0.48
1:F:152:TYR:HD1	2:L:126:ARG:HH21	1.61	0.48
1:A:250:ASP:OD1	1:A:254:ASN:N	2.45	0.48
1:E:39:GLN:CD	1:E:39:GLN:H	2.22	0.48
1:E:308:ASP:OD1	1:E:308:ASP:N	2.44	0.48
2:K:129:GLY:HA2	2:K:221:VAL:O	2.14	0.48
2:K:196:ILE:HD13	2:K:205:ARG:HG2	1.96	0.48
1:D:39:GLN:CD	1:D:39:GLN:H	2.22	0.48
1:D:164:LYS:HG2	1:D:196:LEU:HD21	1.95	0.48
1:C:185:THR:HG22	1:C:342:LEU:HD11	1.96	0.48
1:C:348:LEU:HD21	1:C:359:LEU:HD13	1.95	0.48
1:F:45:ILE:HD11	1:F:97:ILE:HD11	1.96	0.48
1:A:42:LYS:O	1:A:91:ALA:HB1	2.14	0.47
1:C:250:ASP:HA	1:C:359:LEU:HD23	1.96	0.47
1:D:13:VAL:HA	1:D:106:ASP:HA	1.96	0.47
1:F:29:PHE:HD2	1:F:131:MET:HG2	1.80	0.47
2:G:230:VAL:HG12	2:G:237:HIS:HB2	1.95	0.47
2:L:164:ILE:O	2:L:167:THR:HG22	2.15	0.47
1:A:127:ILE:HG22	1:A:131:MET:HE3	1.95	0.47
1:F:150:ASN:N	1:F:150:ASN:OD1	2.47	0.47
2:G:123:MET:HE2	2:G:130:ALA:HB2	1.95	0.47
2:J:154:VAL:O	2:J:155:SER:OG	2.26	0.47
1:C:80:PRO:HG3	1:C:339:GLY:O	2.14	0.47
1:C:161:GLN:HG3	2:H:165:PRO:HB3	1.96	0.47
1:D:185:THR:HG22	1:D:342:LEU:HD11	1.96	0.47
1:A:161:GLN:HG3	2:J:165:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:127:ARG:HD2	2:I:224:GLU:O	2.14	0.47
2:J:207:ALA:O	2:J:210:ILE:HG22	2.14	0.47
1:B:185:THR:HG22	1:B:342:LEU:HD11	1.96	0.47
1:D:28:ARG:HH22	1:D:140:ARG:HG2	1.79	0.47
1:E:171:PHE:HB3	1:E:174:ILE:HD12	1.96	0.47
1:E:237:LEU:HD13	1:E:345:ALA:HB1	1.97	0.47
1:A:89:MET:HE1	1:A:152:TYR:CE2	2.50	0.47
1:B:45:ILE:HD11	1:B:97:ILE:HD11	1.97	0.47
1:E:78:SER:HB2	1:E:80:PRO:HD2	1.96	0.47
2:K:154:VAL:HG22	2:K:181:ILE:HG13	1.97	0.47
1:D:85:LEU:HB3	1:D:89:MET:HE3	1.97	0.47
1:B:296:LYS:HE2	1:B:296:LYS:HB3	1.75	0.47
2:K:111:LYS:O	2:K:112:THR:OG1	2.32	0.47
2:G:164:ILE:HG22	2:G:167:THR:OG1	2.15	0.46
2:H:146:THR:CG2	2:H:187:TYR:H	2.28	0.46
2:I:201:GLY:O	2:I:203:ARG:N	2.47	0.46
1:A:308:ASP:OD1	1:A:308:ASP:N	2.45	0.46
1:C:315:MET:HE2	1:C:333:LEU:HD12	1.97	0.46
1:E:125:ALA:O	1:E:129:ARG:HG3	2.15	0.46
1:F:100:SER:OG	1:F:240:ASP:OD2	2.30	0.46
2:K:158:LEU:O	2:K:162:ILE:HG12	2.15	0.46
2:G:163:PHE:HZ	2:G:174:VAL:HB	1.79	0.46
2:H:246:LYS:HA	2:H:249:LEU:HB2	1.97	0.46
2:J:131:LEU:HD23	2:J:173:ALA:HB2	1.97	0.46
1:B:111:PHE:HB3	1:B:119:LEU:HD13	1.97	0.46
1:E:315:MET:HE2	1:E:333:LEU:HD12	1.96	0.46
1:F:274:ARG:O	1:F:321:ASN:ND2	2.49	0.46
2:G:116:ILE:HD11	2:G:176:MET:HE1	1.96	0.46
2:H:131:LEU:HD22	2:H:203:ARG:HG2	1.97	0.46
2:I:164:ILE:HG22	2:I:167:THR:OG1	2.16	0.46
2:K:188:LEU:HD22	2:K:210:ILE:HG12	1.96	0.46
1:A:172:THR:HA	1:A:197:ASP:O	2.16	0.46
1:B:78:SER:HB2	1:B:80:PRO:HD2	1.97	0.46
1:E:159:TYR:CZ	1:E:163:LEU:HD11	2.50	0.46
1:E:160:LEU:HD11	1:E:192:LEU:HB2	1.97	0.46
2:I:191:SER:HB2	2:I:212:GLU:OE2	2.15	0.46
1:C:78:SER:HB2	1:C:80:PRO:HD2	1.98	0.46
1:D:279:THR:HG22	1:D:300:LYS:HB2	1.98	0.46
2:J:201:GLY:O	2:J:203:ARG:N	2.49	0.46
1:D:29:PHE:HD2	1:D:131:MET:HG2	1.80	0.46
1:D:218:SER:HB2	1:D:247:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LEU:HD13	1:D:345:ALA:HB1	1.98	0.46
1:F:257:ASP:OD1	1:F:260:GLN:HG3	2.16	0.46
2:I:140:MET:HE3	2:I:140:MET:HB3	1.81	0.46
2:G:154:VAL:HG22	2:G:181:ILE:HG13	1.97	0.46
2:G:202:THR:OG1	2:G:203:ARG:N	2.49	0.46
2:I:116:ILE:HD11	2:I:176:MET:HE1	1.98	0.46
2:I:131:LEU:HD11	2:I:207:ALA:HB2	1.98	0.46
1:D:127:ILE:HG22	1:D:131:MET:HE3	1.99	0.45
2:K:127:ARG:HD2	2:K:224:GLU:O	2.15	0.45
2:L:146:THR:CG2	2:L:187:TYR:H	2.30	0.45
1:A:123:GLN:O	1:A:127:ILE:HG13	2.16	0.45
1:A:149:VAL:HG11	1:B:54:HIS:CD2	2.52	0.45
1:A:315:MET:HE2	1:A:333:LEU:HD12	1.98	0.45
1:B:36:LYS:HA	1:B:36:LYS:HD3	1.71	0.45
1:C:152:TYR:HD1	2:H:126:ARG:HH21	1.65	0.45
1:D:42:LYS:H	1:D:92:GLU:CG	2.26	0.45
1:E:296:LYS:HB3	1:E:296:LYS:HE2	1.75	0.45
2:I:132:LEU:HD21	2:I:176:MET:SD	2.56	0.45
2:I:164:ILE:HD12	2:I:164:ILE:HA	1.64	0.45
2:J:112:THR:HG23	2:J:154:VAL:HG11	1.97	0.45
1:D:60:LEU:HD13	1:D:95:VAL:HG11	1.99	0.45
1:A:48:ASP:OD2	1:A:50:ARG:NE	2.49	0.45
1:B:237:LEU:HD13	1:B:345:ALA:HB1	1.98	0.45
2:G:140:MET:HE3	2:G:140:MET:HB3	1.84	0.45
2:G:168:PRO:HB2	2:H:157:GLU:HB3	1.98	0.45
2:J:165:PRO:C	2:J:167:THR:H	2.25	0.45
1:D:45:ILE:HD11	1:D:97:ILE:HD11	1.97	0.45
1:F:260:GLN:NE2	1:F:363:ALA:HB1	2.31	0.45
1:A:159:TYR:CZ	1:A:163:LEU:HD11	2.52	0.45
1:C:218:SER:HB2	1:C:247:ILE:HG12	1.98	0.45
1:F:36:LYS:HD3	1:F:36:LYS:HA	1.66	0.45
1:B:104:VAL:HG21	1:B:210:LEU:HA	1.98	0.45
1:B:172:THR:HA	1:B:197:ASP:O	2.17	0.45
1:C:296:LYS:HB3	1:C:296:LYS:HE2	1.75	0.45
2:G:161:ASN:HD21	2:H:167:THR:HG21	1.81	0.45
2:I:248:MET:HE2	2:I:248:MET:HB2	1.85	0.45
1:A:185:THR:HG22	1:A:342:LEU:HD11	1.97	0.45
2:J:196:ILE:O	2:J:198:LYS:N	2.50	0.45
2:K:123:MET:HE1	2:K:163:PHE:CB	2.25	0.45
1:D:284:VAL:HA	1:D:303:GLN:NE2	2.32	0.44
1:F:85:LEU:HB3	1:F:89:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LYS:HA	1:C:36:LYS:HD3	1.68	0.44
1:C:289:GLY:HA3	1:C:367:GLN:O	2.17	0.44
1:E:348:LEU:HD21	1:E:359:LEU:HD13	2.00	0.44
1:C:279:THR:HG22	1:C:300:LYS:HB2	1.99	0.44
2:K:204:HIS:O	2:K:208:VAL:HG12	2.17	0.44
1:A:28:ARG:HH22	1:A:140:ARG:HG2	1.82	0.44
1:A:171:PHE:CE2	1:A:196:LEU:HD13	2.53	0.44
1:A:296:LYS:HE2	1:A:296:LYS:HB3	1.78	0.44
1:C:159:TYR:CZ	1:C:163:LEU:HD11	2.53	0.44
1:F:174:ILE:HG21	1:F:349:MET:HE1	2.00	0.44
1:D:123:GLN:O	1:D:127:ILE:HG13	2.18	0.44
1:E:185:THR:HG22	1:E:342:LEU:HD11	2.00	0.44
1:D:160:LEU:HD12	1:D:160:LEU:HA	1.88	0.44
1:F:237:LEU:HD13	1:F:345:ALA:HB1	1.99	0.44
2:G:204:HIS:O	2:G:208:VAL:HG12	2.18	0.44
2:J:107:GLU:OE1	2:J:107:GLU:N	2.51	0.44
1:C:45:ILE:HD11	1:C:97:ILE:HD11	2.00	0.43
2:H:140:MET:HE3	2:H:140:MET:HB3	1.79	0.43
1:A:29:PHE:HD2	1:A:131:MET:HG2	1.82	0.43
1:A:195:ASP:OD1	2:I:126:ARG:NH1	2.51	0.43
1:B:289:GLY:HA3	1:B:367:GLN:O	2.18	0.43
1:E:123:GLN:O	1:E:127:ILE:HG13	2.19	0.43
1:E:274:ARG:O	1:E:321:ASN:ND2	2.51	0.43
2:I:152:ALA:HB2	2:J:152:ALA:HB2	2.00	0.43
1:B:348:LEU:HD21	1:B:359:LEU:HD13	1.99	0.43
1:D:296:LYS:HE2	1:D:296:LYS:HB3	1.77	0.43
1:B:28:ARG:HH22	1:B:140:ARG:HG2	1.83	0.43
1:B:123:GLN:O	1:B:127:ILE:HG13	2.18	0.43
1:B:154:GLU:HG2	2:I:187:TYR:OH	2.17	0.43
1:C:100:SER:OG	1:C:240:ASP:OD2	2.34	0.43
1:C:127:ILE:HG22	1:C:131:MET:HE3	2.01	0.43
1:D:31:GLY:O	1:D:35:THR:HB	2.19	0.43
1:C:123:GLN:O	1:C:127:ILE:HG13	2.18	0.43
2:K:152:ALA:HB2	2:L:152:ALA:HB2	1.99	0.43
2:L:132:LEU:HD22	2:L:134:ILE:HG13	2.00	0.43
1:D:100:SER:C	1:D:102:ASN:H	2.27	0.43
1:E:218:SER:HB2	1:E:247:ILE:HG12	2.00	0.43
1:F:250:ASP:HA	1:F:359:LEU:HD23	2.01	0.43
2:G:123:MET:HE1	2:G:163:PHE:CD2	2.54	0.43
1:B:232:ASN:O	1:B:232:ASN:ND2	2.52	0.43
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:ALA:HB2	2:H:152:ALA:HB2	2.00	0.43
2:H:164:ILE:O	2:H:167:THR:HG22	2.18	0.43
2:J:169:LEU:HD12	2:J:184:ALA:HB3	2.01	0.43
2:G:162:ILE:HG21	2:G:174:VAL:CG2	2.48	0.43
2:K:168:PRO:HB2	2:L:157:GLU:HB3	2.01	0.43
1:A:49:THR:HG21	1:A:182:ASN:O	2.18	0.43
1:A:250:ASP:HA	1:A:359:LEU:HD23	2.01	0.43
1:C:349:MET:HE3	1:C:349:MET:HB3	1.93	0.43
2:H:251:ALA:O	2:H:253:PHE:N	2.50	0.43
1:A:100:SER:OG	1:A:240:ASP:OD2	2.36	0.42
2:G:135:GLU:N	2:G:135:GLU:OE1	2.52	0.42
2:G:161:ASN:ND2	2:H:167:THR:HG21	2.34	0.42
2:H:132:LEU:HD22	2:H:134:ILE:HG13	2.00	0.42
2:K:162:ILE:HG21	2:K:174:VAL:CG2	2.48	0.42
1:E:302:VAL:HG21	1:E:320:TYR:HE2	1.84	0.42
2:H:126:ARG:O	2:H:127:ARG:HB2	2.19	0.42
2:K:116:ILE:HD11	2:K:176:MET:HE1	2.01	0.42
2:K:191:SER:HB3	2:K:209:GLY:HA2	2.01	0.42
1:A:127:ILE:O	1:A:131:MET:HG3	2.19	0.42
1:F:123:GLN:O	1:F:127:ILE:HG13	2.19	0.42
1:F:125:ALA:O	1:F:129:ARG:HG3	2.19	0.42
1:F:160:LEU:HD12	1:F:160:LEU:HA	1.87	0.42
2:K:164:ILE:HG22	2:K:167:THR:OG1	2.20	0.42
1:B:308:ASP:OD1	1:B:308:ASP:N	2.46	0.42
1:D:15:ASN:O	1:D:19:THR:HG22	2.19	0.42
2:G:248:MET:HB2	2:G:248:MET:HE2	1.79	0.42
2:H:188:LEU:HG	2:H:210:ILE:HB	2.01	0.42
1:B:218:SER:HB2	1:B:247:ILE:HG12	2.01	0.42
1:B:276:LYS:H	1:B:321:ASN:HB2	1.84	0.42
1:C:152:TYR:CE1	2:H:126:ARG:HB3	2.54	0.42
1:E:127:ILE:HG22	1:E:131:MET:HE3	2.01	0.42
1:F:292:LYS:HD3	1:F:292:LYS:HA	1.90	0.42
2:I:190:LEU:HD13	2:I:205:ARG:HB3	2.02	0.42
1:A:38:LYS:HD3	1:A:39:GLN:N	2.35	0.42
1:C:104:VAL:HG21	1:C:210:LEU:HA	2.01	0.42
2:K:218:THR:HB	2:K:231:ALA:HB3	2.02	0.42
1:E:100:SER:C	1:E:102:ASN:H	2.27	0.42
2:J:160:ILE:O	2:J:164:ILE:HG12	2.20	0.42
2:L:140:MET:HE3	2:L:140:MET:HB3	1.88	0.42
1:D:36:LYS:HA	1:D:36:LYS:HD3	1.69	0.42
1:E:150:ASN:OD1	1:E:150:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLU:HG2	2:K:187:TYR:CE1	2.55	0.42
1:C:125:ALA:O	1:C:129:ARG:HG3	2.20	0.42
1:F:3:LYS:HD2	1:F:3:LYS:HA	1.88	0.42
1:C:187:SER:HA	2:G:127:ARG:NH1	2.35	0.42
1:D:136:ASP:OD2	1:D:140:ARG:NH2	2.48	0.42
2:H:126:ARG:HB2	2:H:128:ILE:HG13	2.02	0.42
2:K:188:LEU:HB3	2:K:210:ILE:HB	2.01	0.42
1:A:3:LYS:HB3	1:A:128:GLU:OE2	2.20	0.41
1:A:276:LYS:H	1:A:321:ASN:HB2	1.83	0.41
1:B:72:MET:HE2	1:B:152:TYR:HB2	2.02	0.41
1:C:79:THR:OG1	1:C:242:ASP:HB2	2.20	0.41
1:D:150:ASN:OD1	1:D:150:ASN:N	2.52	0.41
1:C:171:PHE:CE2	1:C:196:LEU:HD13	2.56	0.41
1:C:308:ASP:OD1	1:C:308:ASP:N	2.43	0.41
2:G:132:LEU:HD21	2:G:176:MET:SD	2.60	0.41
2:I:188:LEU:HD22	2:I:210:ILE:HG12	2.02	0.41
2:J:252:GLU:OE2	2:J:252:GLU:N	2.54	0.41
2:L:158:LEU:HD23	2:L:181:ILE:HD12	2.01	0.41
1:B:125:ALA:O	1:B:129:ARG:HG3	2.20	0.41
1:B:250:ASP:OD1	1:B:254:ASN:N	2.50	0.41
1:C:302:VAL:HG21	1:C:320:TYR:HE2	1.85	0.41
1:F:296:LYS:HB3	1:F:296:LYS:HE2	1.76	0.41
2:H:131:LEU:HD23	2:H:173:ALA:HB2	2.02	0.41
2:H:245:LEU:HD23	2:H:245:LEU:HA	1.86	0.41
1:A:30:GLY:O	1:A:33:VAL:HG12	2.20	0.41
1:B:150:ASN:OD1	1:B:150:ASN:N	2.53	0.41
1:F:15:ASN:O	1:F:19:THR:HG22	2.21	0.41
2:G:174:VAL:HG13	2:G:181:ILE:HG23	2.01	0.41
2:I:168:PRO:HB2	2:J:157:GLU:HB3	2.02	0.41
1:D:22:LEU:O	1:D:26:VAL:HG23	2.21	0.41
1:D:159:TYR:CZ	1:D:163:LEU:HD11	2.55	0.41
2:L:245:LEU:O	2:L:246:LYS:HB3	2.20	0.41
1:F:127:ILE:HG22	1:F:131:MET:HE3	2.01	0.41
1:F:349:MET:HE3	1:F:349:MET:HB3	1.94	0.41
1:A:15:ASN:O	1:A:19:THR:HG22	2.21	0.41
1:A:272:GLU:CD	1:A:274:ARG:HH11	2.28	0.41
1:B:44:LEU:O	1:B:94:GLY:HA2	2.21	0.41
1:B:250:ASP:HA	1:B:359:LEU:HD23	2.03	0.41
1:E:36:LYS:HA	1:E:36:LYS:HD3	1.71	0.41
2:G:107:GLU:HB3	2:G:108:ALA:H	1.70	0.41
1:E:160:LEU:HD12	1:E:160:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:ILE:HD12	2:G:164:ILE:HA	1.68	0.41
2:I:107:GLU:HB3	2:I:108:ALA:H	1.72	0.41
2:I:163:PHE:HZ	2:I:174:VAL:HB	1.86	0.41
2:J:158:LEU:HD23	2:J:181:ILE:HD12	2.03	0.41
2:J:194:PRO:HB2	2:J:195:PHE:H	1.69	0.41
2:L:132:LEU:HD21	2:L:176:MET:SD	2.61	0.41
1:A:79:THR:OG1	1:A:242:ASP:HB2	2.20	0.41
1:A:125:ALA:O	1:A:129:ARG:HG3	2.21	0.41
1:B:288:LEU:HD23	1:B:288:LEU:HA	1.94	0.41
1:E:50:ARG:NH1	1:E:103:PRO:O	2.54	0.41
2:I:133:THR:HB	2:I:175:ILE:HD13	2.03	0.41
2:L:119:ALA:O	2:L:123:MET:HG3	2.21	0.41
1:E:100:SER:O	1:E:102:ASN:N	2.54	0.40
1:A:13:VAL:HG12	1:A:17:GLU:HB2	2.02	0.40
1:C:31:GLY:O	1:C:35:THR:HB	2.21	0.40
1:D:126:GLU:OE2	1:D:129:ARG:NH1	2.54	0.40
1:A:302:VAL:HG21	1:A:320:TYR:HE2	1.86	0.40
1:B:127:ILE:HG22	1:B:131:MET:HE3	2.04	0.40
1:B:174:ILE:HG21	1:B:349:MET:HE1	2.03	0.40
1:F:162:PHE:O	1:F:166:THR:HG23	2.21	0.40
2:L:162:ILE:HG21	2:L:174:VAL:HG11	2.03	0.40
1:F:22:LEU:O	1:F:26:VAL:HG23	2.22	0.40
1:C:157:GLN:NE2	2:G:164:ILE:HG23	2.36	0.40
1:F:111:PHE:HB3	1:F:119:LEU:HD13	2.02	0.40
2:K:163:PHE:CZ	2:K:174:VAL:HB	2.55	0.40
2:L:245:LEU:O	2:L:247:GLU:N	2.52	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	367/464 (79%)	345 (94%)	17 (5%)	5 (1%)	9 34
1	B	365/464 (79%)	342 (94%)	22 (6%)	1 (0%)	36 64
1	C	367/464 (79%)	345 (94%)	20 (5%)	2 (0%)	24 55
1	D	366/464 (79%)	343 (94%)	21 (6%)	2 (0%)	24 55
1	E	366/464 (79%)	343 (94%)	21 (6%)	2 (0%)	24 55
1	F	366/464 (79%)	343 (94%)	21 (6%)	2 (0%)	24 55
2	G	144/167 (86%)	132 (92%)	8 (6%)	4 (3%)	4 23
2	H	140/167 (84%)	125 (89%)	9 (6%)	6 (4%)	2 16
2	I	144/167 (86%)	132 (92%)	10 (7%)	2 (1%)	9 34
2	J	145/167 (87%)	120 (83%)	13 (9%)	12 (8%)	0 6
2	K	144/167 (86%)	132 (92%)	10 (7%)	2 (1%)	9 34
2	L	140/167 (84%)	124 (89%)	12 (9%)	4 (3%)	3 22
All	All	3054/3786 (81%)	2826 (92%)	184 (6%)	44 (1%)	9 34

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	199	GLU
1	A	40	ARG
1	A	100	SER
2	G	187	TYR
2	G	202	THR
2	H	112	THR
2	H	127	ARG
2	H	165	PRO
2	I	202	THR
2	J	154	VAL
2	J	178	ASN
2	J	194	PRO
2	J	197	SER
2	J	198	LYS
2	J	202	THR
2	K	127	ARG
2	K	202	THR
2	L	112	THR
2	L	165	PRO
1	A	3	LYS
1	B	100	SER
1	C	100	SER

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Mol	Chain	Res	Type
1	F	100	SER
2	G	127	ARG
2	H	134	ILE
2	H	252	GLU
2	J	134	ILE
2	J	155	SER
2	J	200	LEU
2	L	134	ILE
2	L	252	GLU
1	D	100	SER
1	E	100	SER
1	A	36	LYS
1	D	101	HIS
1	E	101	HIS
2	I	200	LEU
1	A	101	HIS
1	C	101	HIS
1	F	101	HIS
2	H	246	LYS
2	J	168	PRO
2	G	188	LEU
2	J	196	ILE

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	294/380 (77%)	285 (97%)	9 (3%)	35	55
1	B	293/380 (77%)	288 (98%)	5 (2%)	53	65
1	C	294/380 (77%)	287 (98%)	7 (2%)	43	60
1	D	294/380 (77%)	289 (98%)	5 (2%)	53	65
1	E	294/380 (77%)	289 (98%)	5 (2%)	53	65
1	F	293/380 (77%)	287 (98%)	6 (2%)	48	63
2	G	120/139 (86%)	111 (92%)	9 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	118/139 (85%)	107 (91%)	11 (9%)	8 30
2	I	120/139 (86%)	112 (93%)	8 (7%)	15 40
2	J	121/139 (87%)	98 (81%)	23 (19%)	1 9
2	K	120/139 (86%)	111 (92%)	9 (8%)	12 37
2	L	118/139 (85%)	108 (92%)	10 (8%)	10 32
All	All	2479/3114 (80%)	2372 (96%)	107 (4%)	26 49

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	39	GLN
1	A	49	THR
1	A	72	MET
1	A	90	ASP
1	A	97	ILE
1	A	122	GLU
1	A	149	VAL
1	A	222	GLU
1	B	33	VAL
1	B	35	THR
1	B	122	GLU
1	B	149	VAL
1	B	222	GLU
1	C	33	VAL
1	C	35	THR
1	C	122	GLU
1	C	149	VAL
1	C	150	ASN
1	C	157	GLN
1	C	222	GLU
1	D	33	VAL
1	D	35	THR
1	D	122	GLU
1	D	149	VAL
1	D	222	GLU
1	E	33	VAL
1	E	35	THR
1	E	122	GLU
1	E	149	VAL

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Mol	Chain	Res	Type
1	E	222	GLU
1	F	33	VAL
1	F	35	THR
1	F	122	GLU
1	F	149	VAL
1	F	150	ASN
1	F	222	GLU
2	G	117	THR
2	G	140	MET
2	G	162	ILE
2	G	164	ILE
2	G	167	THR
2	G	174	VAL
2	G	190	LEU
2	G	198	LYS
2	G	230	VAL
2	H	132	LEU
2	H	140	MET
2	H	174	VAL
2	H	188	LEU
2	H	200	LEU
2	H	203	ARG
2	H	220	ILE
2	H	223	GLU
2	H	230	VAL
2	H	243	GLU
2	H	245	LEU
2	I	117	THR
2	I	140	MET
2	I	164	ILE
2	I	167	THR
2	I	174	VAL
2	I	190	LEU
2	I	198	LYS
2	I	230	VAL
2	J	109	GLN
2	J	111	LYS
2	J	114	GLU
2	J	125	LYS
2	J	126	ARG
2	J	132	LEU
2	J	140	MET

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Mol	Chain	Res	Type
2	J	167	THR
2	J	170	HIS
2	J	174	VAL
2	J	188	LEU
2	J	195	PHE
2	J	198	LYS
2	J	199	GLU
2	J	200	LEU
2	J	205	ARG
2	J	217	LEU
2	J	223	GLU
2	J	243	GLU
2	J	245	LEU
2	J	247	GLU
2	J	249	LEU
2	J	252	GLU
2	K	164	ILE
2	K	167	THR
2	K	174	VAL
2	K	190	LEU
2	K	197	SER
2	K	198	LYS
2	K	200	LEU
2	K	230	VAL
2	K	248	MET
2	L	132	LEU
2	L	154	VAL
2	L	162	ILE
2	L	174	VAL
2	L	188	LEU
2	L	200	LEU
2	L	220	ILE
2	L	230	VAL
2	L	243	GLU
2	L	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	191	HIS
1	A	268	HIS

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Mol	Chain	Res	Type
1	B	54	HIS
1	B	232	ASN
1	B	268	HIS
1	B	326	GLN
1	C	157	GLN
1	C	232	ASN
1	D	15	ASN
1	D	326	GLN
1	E	326	GLN
1	F	260	GLN
1	F	326	GLN
2	H	204	HIS
2	K	166	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 oligosaccharides 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	368/464 (79%)	-0.10	0 100 100	47, 89, 122, 146	1 (0%)
1	B	366/464 (78%)	-0.09	0 100 100	54, 101, 136, 150	1 (0%)
1	C	368/464 (79%)	-0.02	3 (0%) 82 59	53, 104, 134, 157	1 (0%)
1	D	367/464 (79%)	-0.05	1 (0%) 90 75	76, 126, 158, 179	1 (0%)
1	E	367/464 (79%)	0.00	0 100 100	64, 117, 149, 168	1 (0%)
1	F	367/464 (79%)	0.09	1 (0%) 90 75	76, 129, 171, 187	1 (0%)
2	G	146/167 (87%)	0.13	0 100 100	27, 80, 115, 168	27 (18%)
2	H	144/167 (86%)	0.20	0 100 100	26, 79, 109, 148	22 (15%)
2	I	146/167 (87%)	0.20	2 (1%) 73 46	35, 82, 113, 131	27 (18%)
2	J	147/167 (88%)	0.13	0 100 100	32, 83, 119, 149	22 (14%)
2	K	146/167 (87%)	0.29	3 (2%) 63 38	42, 94, 124, 144	27 (18%)
2	L	144/167 (86%)	0.14	1 (0%) 84 61	34, 90, 124, 142	22 (15%)
All	All	3076/3786 (81%)	0.03	11 (0%) 88 71	26, 103, 150, 187	153 (4%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	135	GLU	3.1
1	C	191	HIS	2.9
1	C	194	ALA	2.7
2	K	252	GLU	2.4
2	L	201	GLY	2.3
2	I	171	ASP	2.3
1	C	156	GLY	2.1
2	K	107	GLU	2.1
1	D	284	VAL	2.1
2	I	135	GLU	2.1
1	F	104	VAL	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 oligosaccharides 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.