



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:16 PM GMT

PDB ID : 1WYE  
Title : Crystal structure of 2-keto-3-deoxygluconate kinase (form 1) from Sulfolobus Tokodaii  
Authors : Toyoda, T; Suzuki, K.; Hossain, M.T.; Koike, I.; Sekiguchi, T.; Takenaka, A.  
Deposited on : 2005-02-12  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

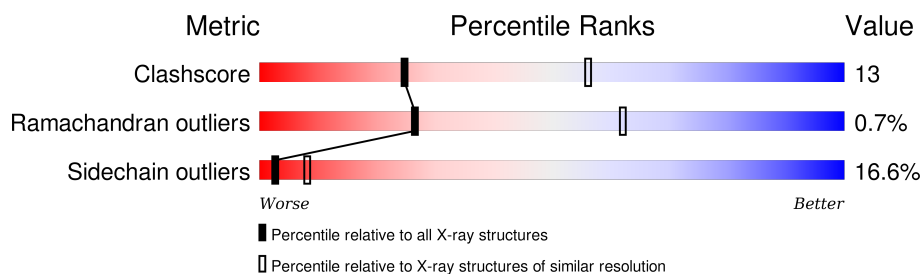
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	
1	C	311	
1	D	311	
1	E	311	
1	F	311	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14836 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 2-keto-3-deoxygluconate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	B	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	C	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	D	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	E	309	Total	C	N	O	S	0	0	0
			2410	1548	389	466	7			
1	F	309	Total	C	N	O	S	0	0	0
			2406	1545	388	466	7			

- Molecule 2 is water.

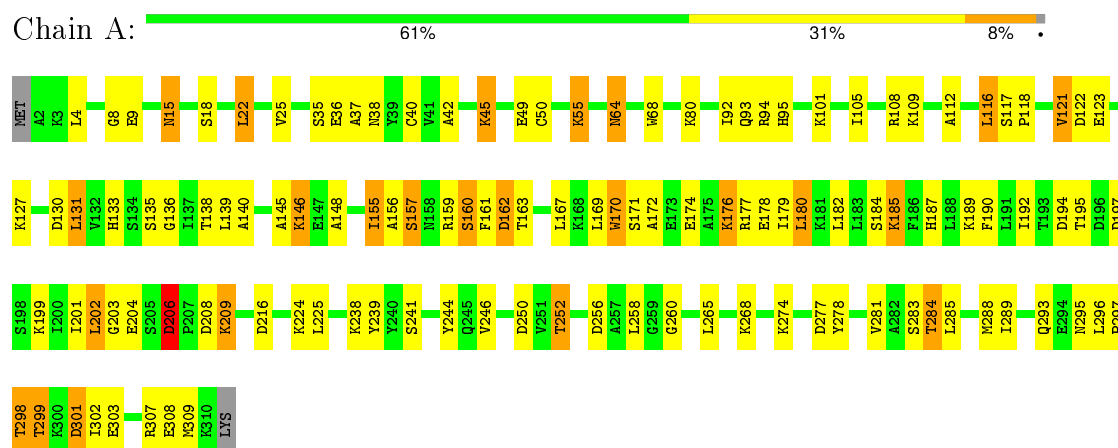
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	45	Total	O	0	0
			45	45		
2	C	71	Total	O	0	0
			71	71		
2	D	79	Total	O	0	0
			79	79		
2	E	76	Total	O	0	0
			76	76		
2	F	54	Total	O	0	0
			54	54		

### 3 Residue-property plots

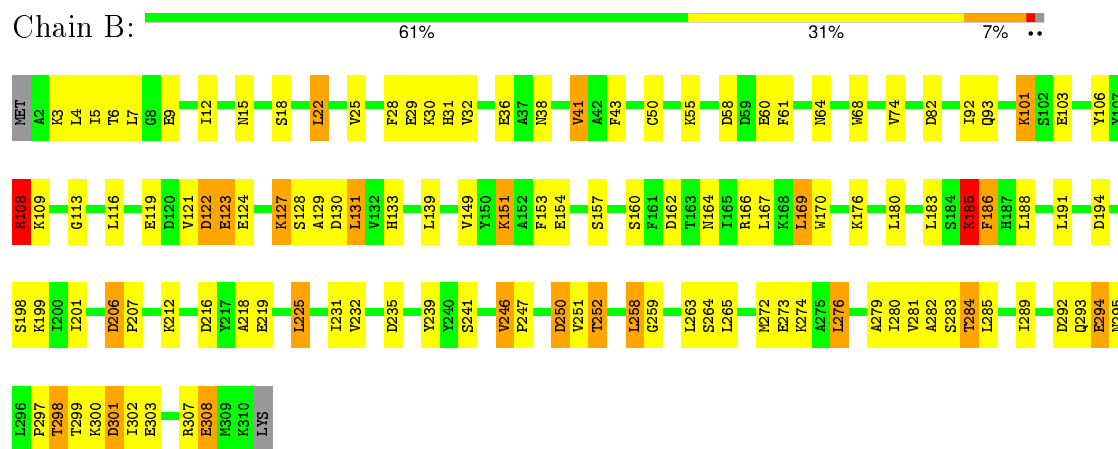
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

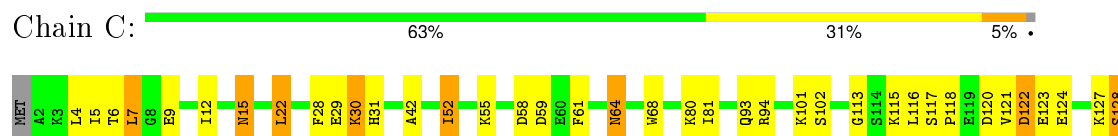
- Molecule 1: 2-keto-3-deoxygluconate kinase

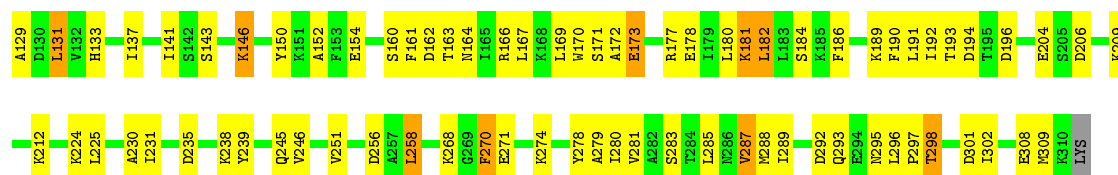


- Molecule 1: 2-keto-3-deoxygluconate kinase



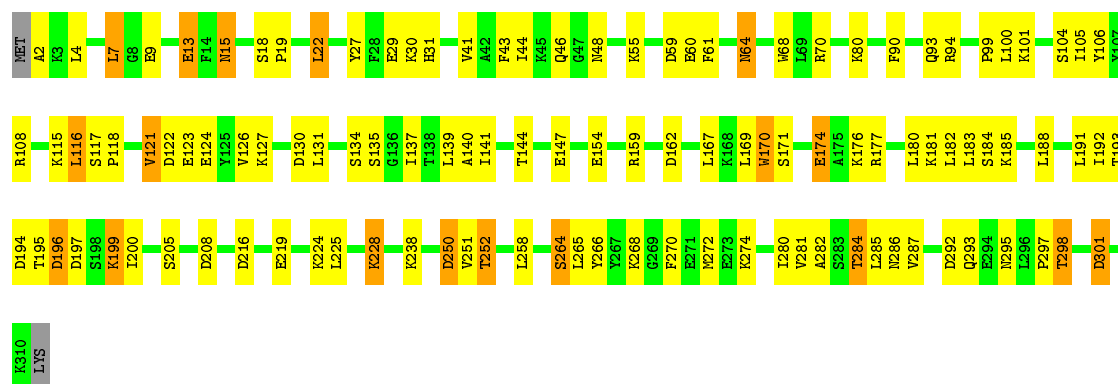
- Molecule 1: 2-keto-3-deoxygluconate kinase





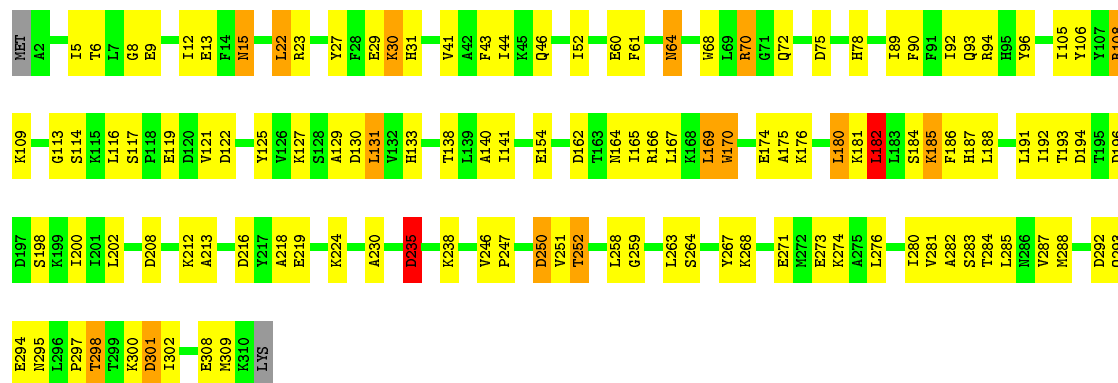
• Molecule 1: 2-keto-3-deoxygluconate kinase

Chain D: 63% 31% 6% •



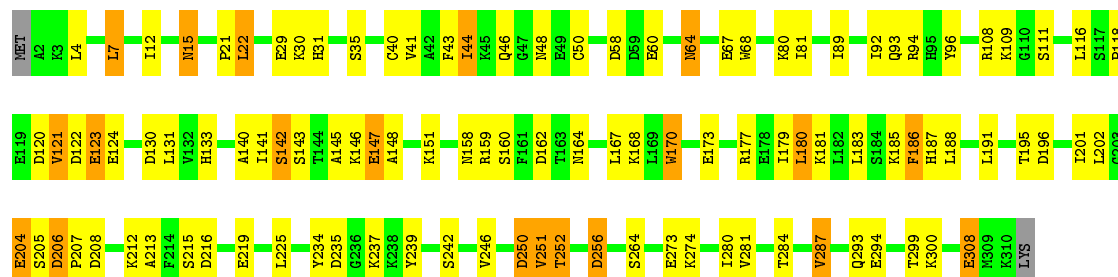
• Molecule 1: 2-keto-3-deoxygluconate kinase

Chain E: 60% 34% 5% ••



• Molecule 1: 2-keto-3-deoxygluconate kinase

Chain F: 65% 28% 6% •



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.67 Å   149.10 Å   161.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.8 (50.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 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	0.77	0/2461	0.94	10/3324 (0.3%)
1	B	0.78	0/2461	0.93	12/3324 (0.4%)
1	C	0.81	0/2461	0.95	7/3324 (0.2%)
1	D	0.80	0/2461	0.97	8/3324 (0.2%)
1	E	0.79	0/2461	0.96	12/3324 (0.4%)
1	F	0.73	0/2457	0.94	8/3320 (0.2%)
All	All	0.78	0/14762	0.95	57/19940 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	ASP	CB-CG-OD2	8.20	125.68	118.30
1	F	162	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	216	ASP	CB-CG-OD2	7.89	125.40	118.30
1	F	250	ASP	CB-CG-OD2	7.87	125.38	118.30
1	A	206	ASP	CB-CG-OD2	7.43	124.99	118.30
1	C	162	ASP	CB-CG-OD2	7.28	124.85	118.30
1	E	130	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	130	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	122	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	197	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	235	ASP	CB-CG-OD2	6.62	124.25	118.30
1	D	197	ASP	CB-CG-OD2	6.58	124.22	118.30
1	F	256	ASP	CB-CG-OD2	6.54	124.19	118.30
1	E	208	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	122	ASP	CB-CG-OD2	6.48	124.13	118.30
1	D	250	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	301	ASP	CB-CG-OD2	6.41	124.07	118.30
1	F	130	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	301	ASP	CB-CG-OD2	6.13	123.82	118.30
1	E	162	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	194	ASP	CB-CG-OD2	6.03	123.73	118.30
1	E	250	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	58	ASP	CB-CG-OD2	5.92	123.62	118.30
1	F	216	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	120	ASP	CB-CG-OD2	5.88	123.60	118.30
1	C	196	ASP	CB-CG-OD2	5.77	123.50	118.30
1	D	162	ASP	CB-CG-OD2	5.73	123.45	118.30
1	E	301	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	130	ASP	CB-CG-OD2	5.71	123.43	118.30
1	B	250	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	58	ASP	CB-CG-OD2	5.70	123.42	118.30
1	E	75	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	196	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	235	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	216	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	208	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	82	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	292	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	162	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	256	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	70	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	F	7	LEU	CA-CB-CG	5.37	127.64	115.30
1	C	122	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	116	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	162	ASP	CB-CG-OD2	5.25	123.02	118.30
1	E	182	LEU	CA-CB-CG	5.25	127.36	115.30
1	B	108	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	277	ASP	CB-CG-OD1	5.21	122.99	118.30
1	F	120	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	59	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	206	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	196	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	194	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	301	ASP	CB-CG-OD2	5.08	122.88	118.30
1	C	59	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	130	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ILE	Peptide
1	F	234	TYR	Peptide

## 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	2410	0	2392	63	0
1	B	2410	0	2392	65	0
1	C	2410	0	2392	61	0
1	D	2410	0	2392	70	0
1	E	2410	0	2392	67	0
1	F	2406	0	2381	57	0
2	A	55	0	0	3	0
2	B	45	0	0	3	0
2	C	71	0	0	3	0
2	D	79	0	0	5	0
2	E	76	0	0	3	0
2	F	54	0	0	2	0
All	All	14836	0	14341	369	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 13.

All (369) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:HE2	1:C:64:ASN:OD1	1.44	1.17
1:E:184:SER:O	1:E:185:LYS:HG2	1.56	1.05
1:A:146:LYS:HE2	1:A:178:GLU:OE1	1.56	1.04
1:A:15:ASN:HD21	1:A:94:ARG:HD3	1.23	1.00
1:D:258:LEU:HD11	1:D:280:ILE:HD13	1.42	1.00
1:B:298:THR:HG22	1:B:301:ASP:H	1.27	1.00
1:C:15:ASN:HD21	1:C:94:ARG:HD3	1.28	0.97
1:D:70:ARG:O	1:E:70:ARG:HD2	1.72	0.90
1:A:68:TRP:HE1	1:A:293:GLN:NE2	1.71	0.89
1:D:298:THR:HG22	1:D:301:ASP:H	1.36	0.88
1:B:6:THR:HG22	1:B:133:HIS:HB3	1.55	0.87
1:C:298:THR:HG22	1:C:301:ASP:H	1.38	0.86
1:B:68:TRP:HE1	1:B:293:GLN:NE2	1.73	0.86
1:A:298:THR:HG22	1:A:301:ASP:H	1.42	0.85
1:E:5:ILE:HD12	1:E:129:ALA:HB2	1.59	0.85
1:A:160:SER:HB2	1:A:190:PHE:HB2	1.56	0.85
1:C:5:ILE:HD12	1:C:129:ALA:HB2	1.60	0.83
1:F:29:GLU:OE2	1:F:31:HIS:HE1	1.61	0.83
1:D:30:LYS:HE3	1:D:64:ASN:OD1	1.79	0.82
1:E:15:ASN:HD21	1:E:94:ARG:HD3	1.42	0.81
1:D:258:LEU:CD1	1:D:280:ILE:HD13	2.09	0.81
1:D:266:TYR:HD2	1:D:272:MET:HE1	1.46	0.81
1:C:127:LYS:O	1:C:128:SER:HB3	1.79	0.80
1:D:30:LYS:CE	1:D:64:ASN:OD1	2.30	0.79
1:E:192:ILE:HG22	1:E:224:LYS:HE2	1.67	0.77
1:D:280:ILE:O	1:D:284:THR:HG22	1.85	0.76
1:D:7:LEU:CD1	1:D:116:LEU:HD11	2.15	0.76
1:D:258:LEU:HD11	1:D:280:ILE:CD1	2.16	0.75
1:E:298:THR:HG22	1:E:301:ASP:H	1.51	0.75
1:F:15:ASN:HD21	1:F:94:ARG:HD3	1.52	0.74
1:B:241:SER:HB3	1:B:276:LEU:HD23	1.69	0.74
1:E:5:ILE:CD1	1:E:129:ALA:HB2	2.18	0.74
1:C:68:TRP:HE1	1:C:293:GLN:NE2	1.85	0.74
1:A:244:TYR:HB2	1:A:284:THR:HG21	1.68	0.74
1:F:280:ILE:O	1:F:284:THR:HG23	1.87	0.73
1:D:280:ILE:O	1:D:284:THR:CG2	2.37	0.72
1:C:124:GLU:HB2	2:C:363:HOH:O	1.90	0.71
1:B:12:ILE:HG13	1:B:61:PHE:HB3	1.73	0.70
1:A:93:GLN:HE22	1:B:60:GLU:HG3	1.55	0.70
1:B:276:LEU:O	1:B:280:ILE:HG12	1.91	0.70
1:E:117:SER:OG	1:E:119:GLU:HG2	1.91	0.70
1:F:12:ILE:HB	1:F:89:ILE:HG22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD13	1:B:93:GLN:HG3	1.73	0.69
1:C:127:LYS:O	1:C:128:SER:CB	2.39	0.69
1:B:68:TRP:HE1	1:B:293:GLN:HE22	1.40	0.69
1:D:29:GLU:OE2	1:D:31:HIS:HE1	1.75	0.69
1:D:7:LEU:HD13	1:D:116:LEU:HD11	1.75	0.69
1:F:187:HIS:HB2	2:F:342:HOH:O	1.93	0.68
1:E:68:TRP:HE1	1:E:293:GLN:NE2	1.90	0.68
1:C:225:LEU:HD11	1:C:231:ILE:HD11	1.75	0.68
1:C:146:LYS:HE2	1:C:178:GLU:OE1	1.94	0.68
1:C:15:ASN:ND2	1:C:94:ARG:HD3	2.08	0.66
1:A:299:THR:O	1:A:303:GLU:HG3	1.96	0.66
1:E:114:SER:HA	1:E:141:ILE:HD12	1.79	0.65
1:B:308:GLU:HB3	2:B:348:HOH:O	1.96	0.65
1:E:298:THR:HG23	2:E:322:HOH:O	1.95	0.64
1:E:250:ASP:OD1	1:E:252:THR:HG23	1.96	0.64
1:D:106:TYR:CD2	1:D:108:ARG:HD2	2.32	0.64
1:D:68:TRP:HE1	1:D:293:GLN:NE2	1.95	0.64
1:E:280:ILE:O	1:E:284:THR:HG23	1.97	0.64
1:F:68:TRP:HE1	1:F:293:GLN:NE2	1.95	0.64
1:B:281:VAL:HA	1:B:284:THR:HG23	1.80	0.64
1:A:22:LEU:HB2	1:A:93:GLN:NE2	2.12	0.64
1:E:247:PRO:HD2	1:E:288:MET:HE3	1.80	0.64
1:C:181:LYS:O	1:C:184:SER:HB2	1.98	0.63
1:A:201:ILE:HG22	1:A:202:LEU:HG	1.80	0.63
1:E:106:TYR:HB3	1:E:108:ARG:HG2	1.80	0.63
1:F:239:TYR:CD2	1:F:273:GLU:HB3	2.34	0.63
1:B:92:ILE:HD13	1:B:252:THR:HG21	1.80	0.62
1:E:93:GLN:HE22	1:F:60:GLU:HG3	1.62	0.62
1:D:281:VAL:HA	1:D:284:THR:HG23	1.81	0.62
1:F:92:ILE:HD13	1:F:252:THR:HG21	1.80	0.62
1:A:22:LEU:HD22	1:A:105:ILE:HD13	1.82	0.62
1:F:204:GLU:OE2	1:F:204:GLU:HA	1.99	0.62
1:D:282:ALA:HA	1:D:297:PRO:HG3	1.82	0.62
1:C:298:THR:HG21	2:C:354:HOH:O	1.99	0.61
1:D:99:PRO:O	1:D:100:LEU:HB2	2.01	0.61
1:F:29:GLU:OE2	1:F:31:HIS:CE1	2.49	0.61
1:D:266:TYR:HD2	1:D:272:MET:CE	2.14	0.61
1:B:298:THR:HG22	1:B:301:ASP:N	2.08	0.61
1:C:298:THR:CG2	1:C:301:ASP:H	2.12	0.61
1:D:199:LYS:HG2	1:D:205:SER:HB3	1.82	0.60
1:A:68:TRP:HE1	1:A:293:GLN:HE22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASN:ND2	1:A:94:ARG:HD3	2.06	0.60
1:A:199:LYS:O	1:A:203:GLY:HA2	2.01	0.60
1:B:297:PRO:HB2	1:B:302:ILE:HG13	1.84	0.60
1:C:55:LYS:HG3	1:C:80:LYS:HB2	1.82	0.60
1:C:172:ALA:HB3	1:C:173:GLU:OE2	2.01	0.59
1:E:46:GLN:HB2	1:E:264:SER:OG	2.02	0.59
1:B:250:ASP:OD1	1:B:252:THR:CG2	2.50	0.59
1:B:101:LYS:HE3	1:F:308:GLU:HG2	1.84	0.59
1:D:137:ILE:O	1:D:141:ILE:HG23	2.02	0.59
1:B:121:VAL:HG22	1:B:151:LYS:HD3	1.85	0.59
1:D:30:LYS:HE2	1:D:64:ASN:OD1	2.01	0.59
1:E:285:LEU:O	1:E:295:ASN:ND2	2.36	0.58
1:C:68:TRP:HE1	1:C:293:GLN:HE21	1.49	0.58
1:A:45:LYS:HD3	1:A:296:LEU:O	2.03	0.58
1:B:29:GLU:OE2	1:B:31:HIS:HE1	1.86	0.58
1:A:55:LYS:HG3	1:A:80:LYS:HB2	1.85	0.58
1:A:35:SER:HA	1:A:256:ASP:OD2	2.04	0.57
1:A:162:ASP:OD1	1:A:224:LYS:NZ	2.33	0.57
1:E:43:PHE:HA	1:E:264:SER:HB2	1.86	0.57
1:A:278:TYR:OH	1:A:303:GLU:OE2	2.17	0.57
1:E:247:PRO:HD2	1:E:288:MET:CE	2.34	0.57
1:E:15:ASN:HD21	1:E:94:ARG:CD	2.15	0.56
1:A:22:LEU:HB2	1:A:93:GLN:HE21	1.69	0.56
1:A:38:ASN:OD1	1:A:293:GLN:HG3	2.06	0.56
1:B:250:ASP:OD1	1:B:252:THR:HG22	2.05	0.56
1:A:281:VAL:HG22	1:A:302:ILE:HG12	1.87	0.56
1:F:250:ASP:OD1	1:F:252:THR:HG23	2.06	0.56
1:C:12:ILE:HG13	1:C:61:PHE:HB3	1.86	0.56
1:B:282:ALA:HA	1:B:297:PRO:HG2	1.87	0.56
1:C:225:LEU:HD11	1:C:231:ILE:CD1	2.35	0.56
1:C:246:VAL:CG1	1:C:288:MET:HG2	2.36	0.56
1:F:121:VAL:O	1:F:151:LYS:HE2	2.05	0.56
1:D:117:SER:HB2	1:D:118:PRO:CD	2.36	0.55
1:C:251:VAL:HG12	1:C:287:VAL:HG22	1.88	0.55
1:B:188:LEU:O	1:B:218:ALA:HA	2.06	0.55
1:A:206:ASP:OD1	1:A:209:LYS:HB2	2.06	0.55
1:A:159:ARG:NH1	1:A:187:HIS:O	2.39	0.55
1:B:36:GLU:HB2	2:B:345:HOH:O	2.05	0.55
1:D:2:ALA:N	1:D:48:ASN:HD22	2.04	0.55
1:A:177:ARG:HH11	1:A:177:ARG:CB	2.20	0.55
1:D:121:VAL:HG23	1:D:126:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:THR:HG22	1:E:133:HIS:HB3	1.89	0.55
1:C:204:GLU:HG2	1:C:209:LYS:HB3	1.89	0.55
1:C:258:LEU:CD2	1:C:280:ILE:HD13	2.37	0.55
1:C:278:TYR:CD2	1:C:302:ILE:HG21	2.42	0.54
1:B:106:TYR:HB3	1:B:108:ARG:HG2	1.88	0.54
1:D:117:SER:HB2	1:D:118:PRO:HD2	1.88	0.54
1:D:106:TYR:HB3	1:D:108:ARG:HG2	1.90	0.54
1:B:299:THR:O	1:B:303:GLU:HG3	2.07	0.54
1:E:202:LEU:HD13	1:E:213:ALA:HB3	1.88	0.54
1:C:258:LEU:HB2	1:C:283:SER:HB3	1.89	0.54
1:C:55:LYS:CG	1:C:80:LYS:HB2	2.37	0.54
1:F:44:ILE:O	1:F:44:ILE:HG13	2.07	0.54
1:E:41:VAL:HA	1:E:44:ILE:HG22	1.88	0.54
1:D:9:GLU:HB3	2:D:385:HOH:O	2.07	0.54
1:F:183:LEU:CD2	1:F:188:LEU:HD11	2.37	0.53
1:B:289:ILE:HG22	1:D:19:PRO:HG2	1.89	0.53
1:C:206:ASP:HB3	1:C:209:LYS:HB2	1.90	0.53
1:D:298:THR:HG22	1:D:301:ASP:N	2.16	0.53
1:D:68:TRP:HE1	1:D:293:GLN:HE21	1.56	0.53
1:E:60:GLU:HG3	1:F:93:GLN:HE22	1.72	0.53
1:D:286:ASN:ND2	2:D:312:HOH:O	2.42	0.53
1:E:13:GLU:HG3	1:E:90:PHE:CZ	2.44	0.53
1:C:164:ASN:OD1	1:C:166:ARG:NH2	2.39	0.53
1:E:284:THR:HG22	2:E:363:HOH:O	2.09	0.52
1:E:22:LEU:H	1:E:93:GLN:NE2	2.07	0.52
1:A:161:PHE:CE2	1:A:163:THR:HA	2.44	0.52
1:C:133:HIS:HA	1:C:160:SER:O	2.08	0.52
1:B:259:GLY:O	1:B:263:LEU:HG	2.09	0.52
1:A:8:GLY:HA2	1:A:138:THR:HG23	1.92	0.52
1:B:22:LEU:HG	1:B:28:PHE:CZ	2.44	0.52
1:A:176:LYS:HE2	1:A:201:ILE:O	2.10	0.52
1:B:176:LYS:HD2	1:B:201:ILE:O	2.09	0.52
1:F:40:CYS:O	1:F:44:ILE:HG22	2.10	0.52
1:A:42:ALA:HB3	1:A:260:GLY:HA3	1.92	0.52
1:B:38:ASN:ND2	1:B:292:ASP:HB3	2.25	0.52
1:A:25:VAL:O	1:B:30:LYS:HE3	2.11	0.51
1:D:224:LYS:HG2	1:D:258:LEU:HD22	1.93	0.51
1:F:133:HIS:HA	1:F:160:SER:O	2.10	0.51
1:D:192:ILE:HG22	1:D:224:LYS:HE2	1.92	0.51
1:B:123:GLU:HG2	1:B:127:LYS:NZ	2.26	0.51
1:D:15:ASN:HD21	1:D:94:ARG:HD3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:VAL:CG2	1:B:151:LYS:HG2	2.41	0.51
1:A:177:ARG:HB3	1:A:177:ARG:NH1	2.25	0.51
1:A:239:TYR:CE2	1:A:241:SER:HB2	2.46	0.51
1:E:68:TRP:HE1	1:E:293:GLN:HE21	1.60	0.50
1:A:145:ALA:O	1:A:148:ALA:HB3	2.11	0.50
1:E:23:ARG:NH1	1:F:67:GLU:OE2	2.39	0.50
1:D:270:PHE:CD1	1:D:274:LYS:HD3	2.46	0.50
1:B:241:SER:OG	1:B:280:ILE:HG13	2.12	0.50
1:B:31:HIS:HD2	1:B:294:GLU:OE2	1.95	0.50
1:E:22:LEU:HD22	1:E:105:ILE:HD13	1.94	0.50
1:C:246:VAL:CG1	1:C:288:MET:CG	2.90	0.50
1:A:250:ASP:OD1	1:A:252:THR:HG23	2.12	0.50
1:F:239:TYR:HD2	1:F:273:GLU:HB3	1.75	0.50
1:C:193:THR:OG1	1:C:194:ASP:N	2.45	0.49
1:D:280:ILE:O	1:D:284:THR:HG23	2.10	0.49
1:D:7:LEU:HD11	1:D:116:LEU:HD11	1.91	0.49
1:D:13:GLU:HB2	1:D:90:PHE:CE1	2.48	0.49
1:E:9:GLU:HG3	1:E:113:GLY:HA3	1.94	0.49
1:A:4:LEU:O	1:A:50:CYS:HA	2.13	0.49
1:D:46:GLN:HE21	1:D:265:LEU:HD21	1.77	0.49
1:F:41:VAL:HG21	1:F:293:GLN:NE2	2.28	0.49
1:D:2:ALA:N	1:D:48:ASN:ND2	2.61	0.49
1:B:32:VAL:HG21	1:B:68:TRP:CB	2.42	0.49
1:F:22:LEU:H	1:F:93:GLN:NE2	2.11	0.49
1:E:297:PRO:HB2	1:E:302:ILE:HG13	1.95	0.49
1:E:78:HIS:HE1	2:E:358:HOH:O	1.96	0.49
1:A:108:ARG:HG3	2:A:316:HOH:O	2.13	0.49
1:E:6:THR:HA	1:E:133:HIS:O	2.13	0.48
1:D:43:PHE:HA	1:D:264:SER:HB2	1.95	0.48
1:B:22:LEU:HG	1:B:28:PHE:HZ	1.79	0.48
1:C:22:LEU:H	1:C:93:GLN:NE2	2.12	0.48
1:B:285:LEU:HD12	1:B:297:PRO:HG3	1.95	0.48
1:E:140:ALA:HB2	1:E:170:TRP:CE2	2.48	0.48
1:D:115:LYS:HE2	2:D:372:HOH:O	2.13	0.48
1:A:204:GLU:OE1	1:A:209:LYS:HD2	2.12	0.48
1:B:108:ARG:HD3	2:B:338:HOH:O	2.14	0.48
1:B:9:GLU:HG3	1:B:113:GLY:HA3	1.95	0.48
1:E:29:GLU:OE1	1:E:31:HIS:HE1	1.96	0.48
1:C:231:ILE:HA	1:C:239:TYR:O	2.14	0.48
1:A:179:ILE:HD13	1:A:201:ILE:HD11	1.96	0.48
1:A:289:ILE:HD11	1:A:295:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:HB3	1:D:144:THR:HB	1.95	0.48
1:E:182:LEU:HD22	1:E:186:PHE:HD1	1.79	0.48
1:F:21:PRO:HG3	1:F:96:TYR:CE1	2.49	0.47
1:F:251:VAL:HG23	1:F:287:VAL:HG22	1.95	0.47
1:F:35:SER:HA	1:F:256:ASP:OD2	2.14	0.47
1:D:104:SER:C	1:D:105:ILE:HD13	2.35	0.47
1:E:165:ILE:HG21	1:E:200:ILE:HD13	1.96	0.47
1:C:258:LEU:HD21	1:C:280:ILE:HD13	1.96	0.47
1:A:297:PRO:HA	1:E:96:TYR:OH	2.15	0.47
1:A:155:ILE:HG22	1:A:155:ILE:O	2.13	0.47
1:E:27:TYR:CE2	1:F:29:GLU:HG3	2.49	0.47
1:A:185:LYS:H	1:A:185:LYS:HD2	1.78	0.47
1:B:225:LEU:HD21	1:B:231:ILE:HD11	1.96	0.47
1:F:58:ASP:HB2	1:F:81:ILE:CG2	2.45	0.47
1:A:117:SER:HB2	1:A:118:PRO:HD2	1.97	0.47
1:B:5:ILE:HD12	1:B:129:ALA:HB2	1.96	0.47
1:E:166:ARG:HB2	1:E:169:LEU:HD22	1.96	0.47
1:E:182:LEU:HD22	1:E:186:PHE:CD1	2.50	0.46
1:B:166:ARG:HB2	1:B:169:LEU:HD22	1.97	0.46
1:B:280:ILE:O	1:B:283:SER:HB3	2.16	0.46
1:C:163:THR:CG2	1:C:193:THR:HB	2.45	0.46
1:D:122:ASP:O	1:D:126:VAL:HG23	2.15	0.46
1:A:37:ALA:O	1:A:40:CYS:HB2	2.14	0.46
1:B:31:HIS:CD2	1:B:294:GLU:OE2	2.68	0.46
1:F:48:ASN:HD22	1:F:48:ASN:HA	1.56	0.46
1:C:289:ILE:HD11	1:C:295:ASN:HB2	1.98	0.46
1:F:21:PRO:HG3	1:F:96:TYR:CZ	2.50	0.46
1:B:231:ILE:HA	1:B:239:TYR:O	2.15	0.46
1:E:164:ASN:OD1	1:E:166:ARG:NH2	2.38	0.46
1:F:145:ALA:O	1:F:148:ALA:HB3	2.16	0.46
1:D:251:VAL:HG23	2:D:373:HOH:O	2.14	0.46
1:A:36:GLU:OE2	1:A:135:SER:HB3	2.16	0.46
1:F:180:LEU:HD13	1:F:201:ILE:CG2	2.46	0.46
1:C:171:SER:HB2	1:C:173:GLU:HG2	1.97	0.46
1:C:137:ILE:O	1:C:141:ILE:HG23	2.16	0.46
1:C:29:GLU:OE2	1:C:31:HIS:HE1	1.99	0.46
1:C:9:GLU:HG3	1:C:113:GLY:HA3	1.96	0.46
1:A:8:GLY:HA2	1:A:138:THR:CG2	2.46	0.46
1:F:206:ASP:HA	1:F:207:PRO:HD2	1.81	0.46
1:A:64:ASN:HD22	1:A:64:ASN:C	2.16	0.46
1:B:149:VAL:O	1:B:153:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLN:NE2	1:F:60:GLU:HG3	2.28	0.45
1:A:118:PRO:HA	1:A:121:VAL:HG13	1.97	0.45
1:C:154:GLU:HB3	1:C:186:PHE:HE2	1.82	0.45
1:B:4:LEU:HD12	1:B:131:LEU:O	2.15	0.45
1:C:6:THR:HA	1:C:133:HIS:O	2.17	0.45
1:C:285:LEU:HD12	1:C:297:PRO:HG3	1.97	0.45
1:F:30:LYS:HE2	1:F:30:LYS:HB3	1.69	0.45
1:F:177:ARG:O	1:F:181:LYS:HB2	2.16	0.45
1:D:171:SER:OG	1:D:174:GLU:HB2	2.17	0.45
1:E:235:ASP:O	1:E:235:ASP:CG	2.54	0.45
1:C:7:LEU:HD11	1:C:152:ALA:HB3	1.97	0.45
1:D:55:LYS:HG3	1:D:80:LYS:HB2	1.98	0.45
1:D:41:VAL:HA	1:D:44:ILE:HG22	1.99	0.45
1:F:4:LEU:O	1:F:50:CYS:HA	2.16	0.45
1:D:250:ASP:OD1	1:D:252:THR:CG2	2.65	0.45
1:E:259:GLY:O	1:E:263:LEU:HG	2.17	0.45
1:E:30:LYS:HG3	1:E:31:HIS:N	2.30	0.44
1:E:165:ILE:HG12	1:E:175:ALA:HB1	1.99	0.44
1:F:159:ARG:HD3	1:F:186:PHE:HB3	1.99	0.44
1:C:101:LYS:HD3	2:C:360:HOH:O	2.15	0.44
1:A:189:LYS:NZ	2:A:318:HOH:O	2.49	0.44
1:C:93:GLN:HE22	1:D:60:GLU:HG3	1.82	0.44
1:D:134:SER:OG	1:D:135:SER:N	2.49	0.44
1:B:41:VAL:HG11	1:B:293:GLN:NE2	2.32	0.44
1:D:121:VAL:HA	2:D:313:HOH:O	2.16	0.44
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.79	0.44
1:B:232:VAL:HB	1:B:276:LEU:HD13	2.00	0.44
1:F:118:PRO:HG3	1:F:147:GLU:HB3	2.00	0.44
1:A:131:LEU:HD11	1:A:160:SER:HB3	2.00	0.44
1:B:123:GLU:H	1:B:123:GLU:CD	2.20	0.44
1:D:225:LEU:HB3	1:D:228:LYS:HB2	1.99	0.44
1:A:140:ALA:HB2	1:A:170:TRP:CE2	2.53	0.44
1:A:136:GLY:HA3	1:A:163:THR:O	2.18	0.44
1:B:55:LYS:O	1:B:113:GLY:HA2	2.17	0.43
1:C:189:LYS:HD3	1:C:190:PHE:CE1	2.52	0.43
1:E:12:ILE:HG13	1:E:61:PHE:HB3	2.00	0.43
1:B:185:LYS:HG2	1:B:185:LYS:H	1.31	0.43
1:D:61:PHE:O	1:D:64:ASN:HB3	2.18	0.43
1:B:206:ASP:OD1	1:B:207:PRO:HD2	2.18	0.43
1:F:183:LEU:HD22	1:F:188:LEU:HD11	2.01	0.43
1:E:198:SER:O	1:E:202:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD11	1:A:133:HIS:HB3	1.99	0.43
1:B:43:PHE:HA	1:B:264:SER:HB2	1.99	0.43
1:E:193:THR:OG1	1:E:194:ASP:N	2.51	0.43
1:A:265:LEU:HD21	1:A:299:THR:HG23	2.01	0.43
1:F:108:ARG:O	1:F:111:SER:HB3	2.19	0.43
1:D:176:LYS:HD3	1:D:200:ILE:O	2.19	0.43
1:C:30:LYS:CE	1:C:64:ASN:OD1	2.38	0.43
1:C:230:ALA:HB3	1:C:280:ILE:HD11	2.01	0.43
1:D:104:SER:O	1:D:105:ILE:HD13	2.18	0.43
1:F:141:ILE:O	1:F:142:SER:HB3	2.19	0.43
1:C:28:PHE:O	1:D:27:TYR:HA	2.19	0.43
1:B:246:VAL:HG22	1:B:247:PRO:HD2	2.00	0.43
1:F:212:LYS:O	1:F:215:SER:OG	2.33	0.43
1:C:235:ASP:CG	1:C:235:ASP:O	2.56	0.43
1:F:179:ILE:O	1:F:183:LEU:HG	2.19	0.43
1:D:4:LEU:HD22	1:D:43:PHE:CD1	2.54	0.43
1:A:171:SER:O	1:A:172:ALA:C	2.57	0.43
1:A:285:LEU:O	1:A:288:MET:HG2	2.19	0.43
1:E:282:ALA:HA	1:E:297:PRO:HG3	2.00	0.43
1:D:4:LEU:HB2	1:D:43:PHE:CE2	2.54	0.43
1:D:140:ALA:HB2	1:D:170:TRP:CE2	2.54	0.43
1:F:43:PHE:CE2	1:F:48:ASN:HB3	2.54	0.42
1:F:140:ALA:HB2	1:F:170:TRP:CE2	2.54	0.42
1:B:133:HIS:HA	1:B:160:SER:O	2.20	0.42
1:F:15:ASN:HD21	1:F:94:ARG:CD	2.27	0.42
1:F:15:ASN:N	1:F:29:GLU:O	2.45	0.42
1:E:250:ASP:OD1	1:E:252:THR:CG2	2.66	0.42
1:F:239:TYR:N	1:F:239:TYR:CD1	2.87	0.42
1:E:230:ALA:HB3	1:E:276:LEU:HD11	2.02	0.42
1:B:92:ILE:HD13	1:B:252:THR:CG2	2.46	0.42
1:D:297:PRO:HA	1:F:96:TYR:OH	2.20	0.42
1:A:55:LYS:HB3	1:A:112:ALA:O	2.20	0.42
1:C:161:PHE:CE2	1:C:163:THR:HA	2.54	0.42
1:A:92:ILE:HG22	1:A:94:ARG:HG2	2.00	0.42
1:B:121:VAL:O	1:B:121:VAL:CG2	2.68	0.42
1:C:270:PHE:CD2	1:C:270:PHE:N	2.88	0.42
1:F:168:LYS:NZ	2:F:365:HOH:O	2.29	0.42
1:A:156:ALA:O	1:A:157:SER:CB	2.67	0.42
1:E:41:VAL:HG21	1:E:72:GLN:HG3	2.02	0.42
1:A:155:ILE:O	1:A:155:ILE:CG2	2.68	0.42
1:A:176:LYS:O	1:A:180:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:LEU:HD13	1:E:93:GLN:HG3	2.02	0.42
1:E:29:GLU:OE1	1:E:31:HIS:CE1	2.73	0.42
1:C:4:LEU:HD13	1:C:131:LEU:HB3	2.01	0.42
1:F:46:GLN:NE2	1:F:299:THR:OG1	2.53	0.42
1:E:187:HIS:CE1	1:E:219:GLU:HG3	2.55	0.42
1:D:123:GLU:OE1	1:D:123:GLU:N	2.53	0.42
1:D:22:LEU:HD13	1:D:93:GLN:CB	2.50	0.42
1:B:22:LEU:HA	1:B:25:VAL:CG2	2.50	0.41
1:B:250:ASP:OD1	1:B:252:THR:HG23	2.20	0.41
1:E:64:ASN:HD22	1:E:64:ASN:C	2.23	0.41
1:C:42:ALA:HA	1:C:296:LEU:HD13	2.02	0.41
1:C:194:ASP:HB3	1:C:224:LYS:HB2	2.01	0.41
1:E:78:HIS:CD2	1:E:125:TYR:CE2	3.08	0.41
1:E:8:GLY:HA2	1:E:138:THR:HG23	2.01	0.41
1:C:150:TYR:CE1	1:C:182:LEU:HD23	2.56	0.41
1:E:22:LEU:H	1:E:93:GLN:HE21	1.67	0.41
1:B:258:LEU:HD13	1:B:279:ALA:HB1	2.01	0.41
1:B:121:VAL:HG22	1:B:151:LYS:CD	2.48	0.41
1:F:202:LEU:HD13	1:F:213:ALA:HB3	2.02	0.41
1:E:176:LYS:O	1:E:180:LEU:HB2	2.20	0.41
1:B:50:CYS:SG	1:B:74:VAL:HG13	2.60	0.41
1:D:258:LEU:CD1	1:D:280:ILE:CD1	2.89	0.41
1:E:92:ILE:HD13	1:E:252:THR:HG21	2.03	0.41
1:C:258:LEU:HD13	1:C:279:ALA:HB1	2.03	0.41
1:F:22:LEU:HD12	1:F:22:LEU:HA	1.86	0.41
1:D:193:THR:OG1	1:D:194:ASP:N	2.54	0.41
1:E:188:LEU:O	1:E:218:ALA:HA	2.21	0.41
1:D:285:LEU:C	1:D:295:ASN:HD22	2.24	0.41
1:F:64:ASN:C	1:F:64:ASN:HD22	2.24	0.41
1:F:80:LYS:HA	1:F:80:LYS:HD3	1.92	0.41
1:A:95:HIS:N	1:A:95:HIS:CD2	2.89	0.40
1:A:298:THR:HG23	2:A:322:HOH:O	2.21	0.40
1:D:13:GLU:HG2	1:D:31:HIS:HB2	2.04	0.40
1:B:154:GLU:HB3	1:B:186:PHE:HE2	1.86	0.40
1:D:183:LEU:HD22	1:D:188:LEU:HD11	2.04	0.40
1:C:117:SER:HB2	1:C:118:PRO:HD2	2.03	0.40
1:F:31:HIS:HD2	1:F:294:GLU:OE2	2.05	0.40
1:C:6:THR:OG1	1:C:52:ILE:CG1	2.69	0.40
1:C:163:THR:HG23	1:C:193:THR:HB	2.04	0.40
1:E:131:LEU:HG	1:E:267:TYR:OH	2.21	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	307/311 (99%)	283 (92%)	22 (7%)	2 (1%)	26	62
1	B	307/311 (99%)	292 (95%)	12 (4%)	3 (1%)	19	52
1	C	307/311 (99%)	295 (96%)	11 (4%)	1 (0%)	46	79
1	D	307/311 (99%)	291 (95%)	16 (5%)	0	100	100
1	E	307/311 (99%)	293 (95%)	11 (4%)	3 (1%)	19	52
1	F	307/311 (99%)	284 (92%)	19 (6%)	4 (1%)	15	44
All	All	1842/1866 (99%)	1738 (94%)	91 (5%)	13 (1%)	26	62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	PHE
1	C	128	SER
1	E	185	LYS
1	F	142	SER
1	F	186	PHE
1	F	287	VAL
1	A	157	SER
1	B	185	LYS
1	A	184	SER
1	B	151	LYS
1	E	235	ASP
1	E	22	LEU
1	F	123	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	257/260 (99%)	211 (82%)	46 (18%)	2	6
1	B	257/260 (99%)	208 (81%)	49 (19%)	2	5
1	C	257/260 (99%)	217 (84%)	40 (16%)	3	9
1	D	257/260 (99%)	216 (84%)	41 (16%)	3	9
1	E	257/260 (99%)	218 (85%)	39 (15%)	3	10
1	F	256/260 (98%)	215 (84%)	41 (16%)	3	9
All	All	1541/1560 (99%)	1285 (83%)	256 (17%)	3	8

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	15	ASN
1	A	18	SER
1	A	22	LEU
1	A	45	LYS
1	A	49	GLU
1	A	55	LYS
1	A	64	ASN
1	A	101	LYS
1	A	109	LYS
1	A	116	LEU
1	A	121	VAL
1	A	123	GLU
1	A	127	LYS
1	A	131	LEU
1	A	139	LEU
1	A	146	LYS
1	A	160	SER
1	A	167	LEU
1	A	169	LEU
1	A	170	TRP
1	A	174	GLU
1	A	176	LYS
1	A	180	LEU
1	A	182	LEU
1	A	185	LYS
1	A	192	ILE

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Mol	Chain	Res	Type
1	A	195	THR
1	A	202	LEU
1	A	206	ASP
1	A	208	ASP
1	A	209	LYS
1	A	225	LEU
1	A	238	LYS
1	A	246	VAL
1	A	252	THR
1	A	258	LEU
1	A	268	LYS
1	A	274	LYS
1	A	283	SER
1	A	284	THR
1	A	298	THR
1	A	299	THR
1	A	307	ARG
1	A	308	GLU
1	A	309	MET
1	B	3	LYS
1	B	7	LEU
1	B	15	ASN
1	B	18	SER
1	B	22	LEU
1	B	41	VAL
1	B	64	ASN
1	B	101	LYS
1	B	103	GLU
1	B	108	ARG
1	B	109	LYS
1	B	116	LEU
1	B	119	GLU
1	B	122	ASP
1	B	123	GLU
1	B	124	GLU
1	B	127	LYS
1	B	128	SER
1	B	131	LEU
1	B	139	LEU
1	B	157	SER
1	B	164	ASN
1	B	167	LEU

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Mol	Chain	Res	Type
1	B	169	LEU
1	B	170	TRP
1	B	183	LEU
1	B	185	LYS
1	B	191	LEU
1	B	198	SER
1	B	199	LYS
1	B	212	LYS
1	B	216	ASP
1	B	219	GLU
1	B	225	LEU
1	B	246	VAL
1	B	251	VAL
1	B	252	THR
1	B	258	LEU
1	B	272	MET
1	B	273	GLU
1	B	274	LYS
1	B	276	LEU
1	B	284	THR
1	B	294	GLU
1	B	295	ASN
1	B	298	THR
1	B	300	LYS
1	B	307	ARG
1	B	308	GLU
1	C	7	LEU
1	C	15	ASN
1	C	22	LEU
1	C	30	LYS
1	C	52	ILE
1	C	64	ASN
1	C	81	ILE
1	C	102	SER
1	C	115	LYS
1	C	116	LEU
1	C	121	VAL
1	C	122	ASP
1	C	123	GLU
1	C	131	LEU
1	C	143	SER
1	C	146	LYS

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Mol	Chain	Res	Type
1	C	167	LEU
1	C	169	LEU
1	C	170	TRP
1	C	173	GLU
1	C	177	ARG
1	C	180	LEU
1	C	181	LYS
1	C	182	LEU
1	C	191	LEU
1	C	192	ILE
1	C	212	LYS
1	C	238	LYS
1	C	245	GLN
1	C	258	LEU
1	C	268	LYS
1	C	270	PHE
1	C	271	GLU
1	C	274	LYS
1	C	281	VAL
1	C	287	VAL
1	C	292	ASP
1	C	298	THR
1	C	308	GLU
1	C	309	MET
1	D	7	LEU
1	D	13	GLU
1	D	15	ASN
1	D	18	SER
1	D	22	LEU
1	D	64	ASN
1	D	101	LYS
1	D	116	LEU
1	D	121	VAL
1	D	124	GLU
1	D	127	LYS
1	D	131	LEU
1	D	139	LEU
1	D	147	GLU
1	D	154	GLU
1	D	159	ARG
1	D	167	LEU
1	D	169	LEU

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Mol	Chain	Res	Type
1	D	170	TRP
1	D	174	GLU
1	D	177	ARG
1	D	180	LEU
1	D	181	LYS
1	D	182	LEU
1	D	184	SER
1	D	185	LYS
1	D	191	LEU
1	D	195	THR
1	D	196	ASP
1	D	199	LYS
1	D	216	ASP
1	D	219	GLU
1	D	228	LYS
1	D	238	LYS
1	D	252	THR
1	D	264	SER
1	D	268	LYS
1	D	284	THR
1	D	287	VAL
1	D	292	ASP
1	D	298	THR
1	E	15	ASN
1	E	30	LYS
1	E	52	ILE
1	E	64	ASN
1	E	89	ILE
1	E	108	ARG
1	E	109	LYS
1	E	116	LEU
1	E	121	VAL
1	E	127	LYS
1	E	131	LEU
1	E	154	GLU
1	E	167	LEU
1	E	169	LEU
1	E	170	TRP
1	E	174	GLU
1	E	180	LEU
1	E	181	LYS
1	E	182	LEU

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Mol	Chain	Res	Type
1	E	191	LEU
1	E	212	LYS
1	E	235	ASP
1	E	238	LYS
1	E	246	VAL
1	E	251	VAL
1	E	252	THR
1	E	258	LEU
1	E	268	LYS
1	E	271	GLU
1	E	273	GLU
1	E	274	LYS
1	E	281	VAL
1	E	283	SER
1	E	287	VAL
1	E	294	GLU
1	E	298	THR
1	E	300	LYS
1	E	308	GLU
1	E	309	MET
1	F	7	LEU
1	F	15	ASN
1	F	22	LEU
1	F	44	ILE
1	F	64	ASN
1	F	109	LYS
1	F	116	LEU
1	F	121	VAL
1	F	122	ASP
1	F	123	GLU
1	F	124	GLU
1	F	131	LEU
1	F	143	SER
1	F	146	LYS
1	F	147	GLU
1	F	158	ASN
1	F	164	ASN
1	F	167	LEU
1	F	170	TRP
1	F	173	GLU
1	F	180	LEU
1	F	185	LYS

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Mol	Chain	Res	Type
1	F	191	LEU
1	F	195	THR
1	F	196	ASP
1	F	204	GLU
1	F	205	SER
1	F	206	ASP
1	F	208	ASP
1	F	219	GLU
1	F	225	LEU
1	F	237	LYS
1	F	242	SER
1	F	246	VAL
1	F	251	VAL
1	F	252	THR
1	F	264	SER
1	F	274	LYS
1	F	281	VAL
1	F	300	LYS
1	F	308	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	31	HIS
1	A	46	GLN
1	A	48	ASN
1	A	78	HIS
1	A	93	GLN
1	A	164	ASN
1	A	286	ASN
1	A	293	GLN
1	B	15	ASN
1	B	31	HIS
1	B	48	ASN
1	B	93	GLN
1	B	95	HIS
1	B	286	ASN
1	B	293	GLN
1	C	15	ASN
1	C	31	HIS
1	C	46	GLN

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Mol	Chain	Res	Type
1	C	48	ASN
1	C	78	HIS
1	C	93	GLN
1	C	286	ASN
1	C	293	GLN
1	D	15	ASN
1	D	31	HIS
1	D	46	GLN
1	D	93	GLN
1	D	286	ASN
1	D	293	GLN
1	D	295	ASN
1	E	15	ASN
1	E	31	HIS
1	E	46	GLN
1	E	48	ASN
1	E	78	HIS
1	E	93	GLN
1	E	286	ASN
1	E	293	GLN
1	F	15	ASN
1	F	31	HIS
1	F	46	GLN
1	F	48	ASN
1	F	93	GLN
1	F	95	HIS
1	F	286	ASN
1	F	293	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 carbohydrates 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.