Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 05:42 AM EDT

PDB ID	:	5H9D
Title	:	Crystal structure of Heptaprenyl Diphosphate Synthase from Staphylococcus aureus
Authors	:	Wei, H.L.; Liu, W.D.; Zheng, Y.Y.; Ko, T.P.; Chen, C.C.; Guo, R.T.
Deposited on	:	2015-12-28
Resolution	:	2.68 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:

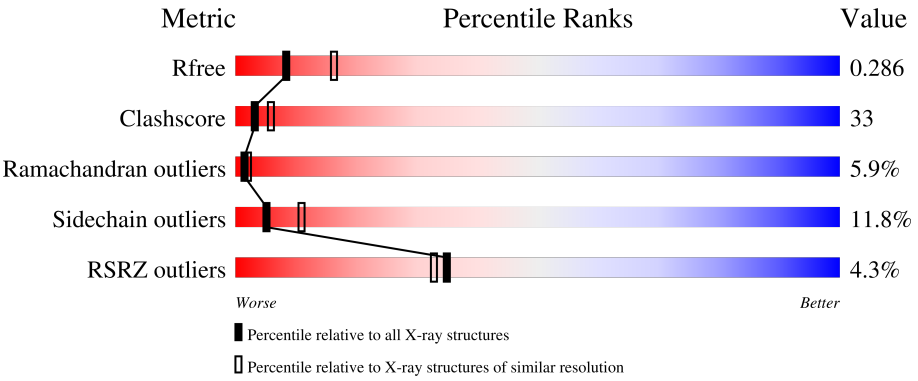
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	319	2% 60% 33% 7%
1	B	319	2% 58% 34% 7%
2	C	190	7% 37% 47% 13%
2	D	190	8% 34% 49% 13%
3	K	17	12% 41% 18% 41%

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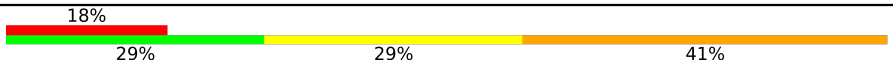
Mol	Chain	Length	Quality of chain
3	L	17	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8584 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 Farnesyl pyrophosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2528	1590	448	481	9			
1	B	318	Total	C	N	O	S	0	0	0
			2528	1590	448	481	9			

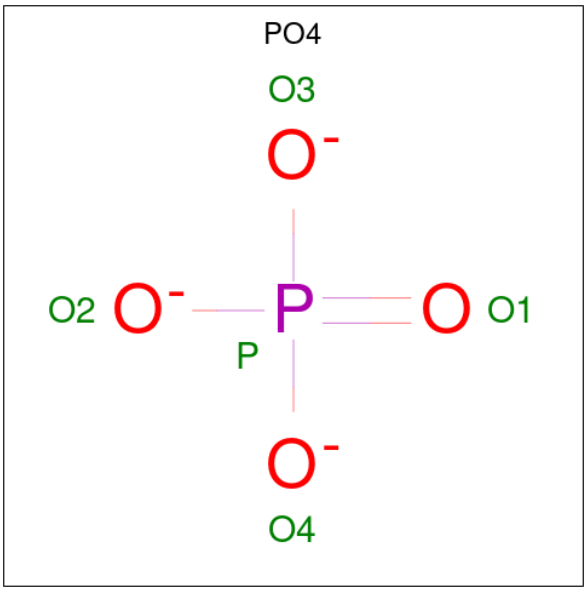
- Molecule 2 is a protein called Heptaprenyl diphosphate synthase (HEPPP synthase) subunit 1 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	188	Total	C	N	O	S	0	0	0
			1547	987	253	304	3			
2	D	188	Total	C	N	O	S	0	0	0
			1547	987	253	304	3			

- Molecule 3 is a protein called C-terminal peptide from Heptaprenyl diphosphate synthase (HEPPP synthase) subunit 1 family protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	17	Total	C	N	O	0	0	0
			148	93	29	26			
3	L	17	Total	C	N	O	0	0	0
			148	93	29	26			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	K	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

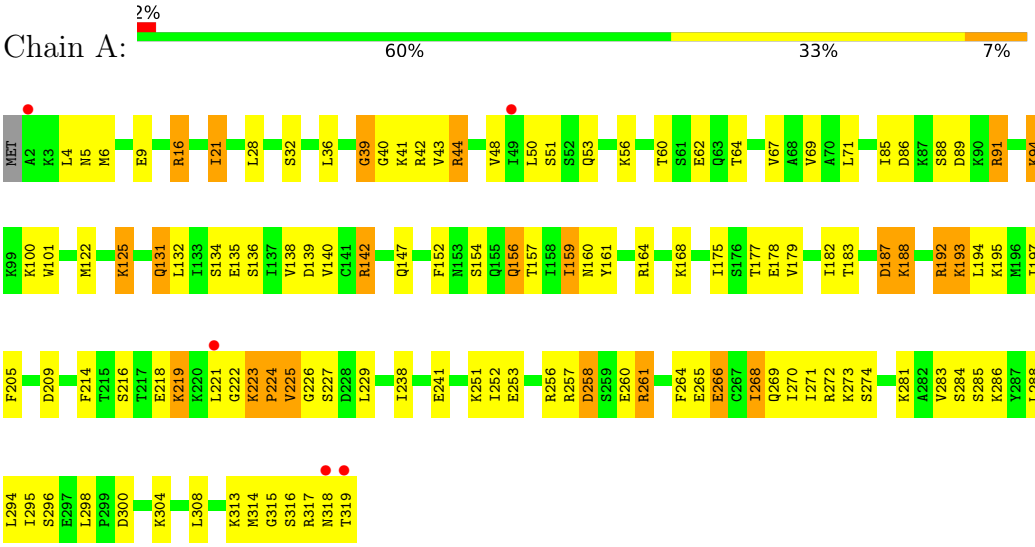
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0
5	B	26	Total O 26 26	0	0
5	C	20	Total O 20 20	0	0
5	D	19	Total O 19 19	0	0
5	K	17	Total O 17 17	0	0
5	L	15	Total O 15 15	0	0

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.

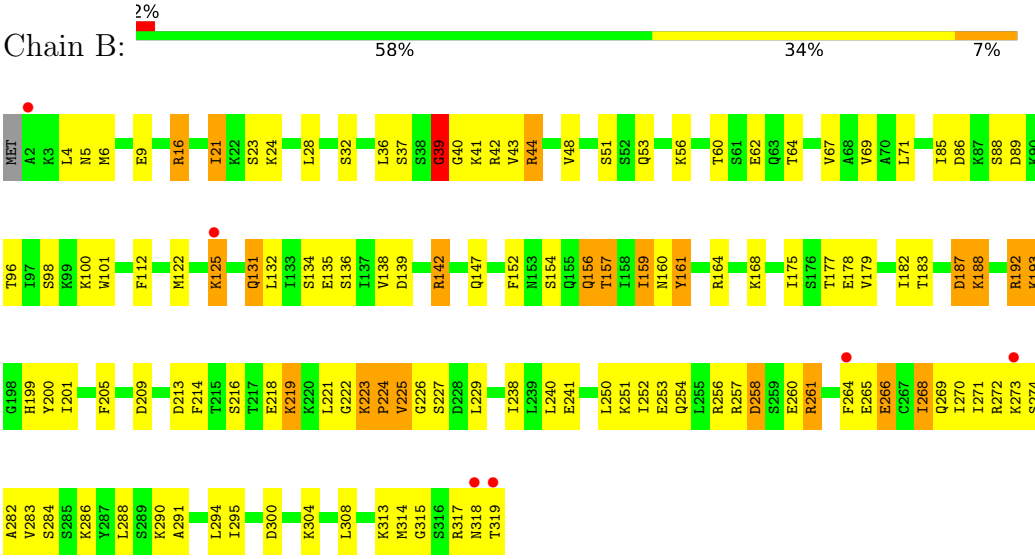
• Molecule 1: Farnesyl pyrophosphate synthetase

Chain A:



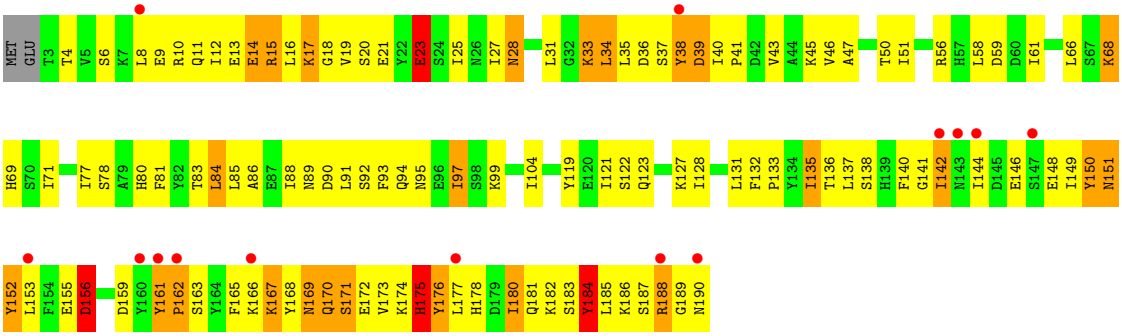
• Molecule 1: Farnesyl pyrophosphate synthetase

Chain B:

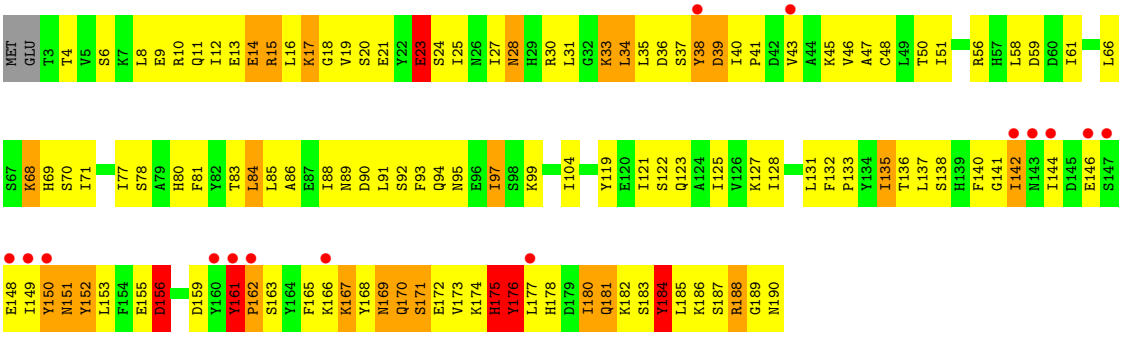


• Molecule 2: Heptaprenyl diphosphate synthase (HEPPP synthase) subunit 1 family protein

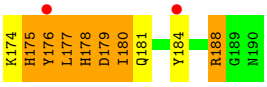
Chain C:



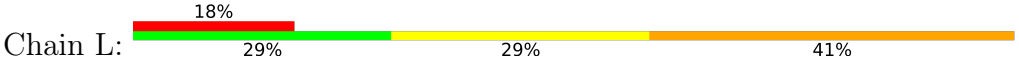
• Molecule 2: Heptaprenyl diphosphate synthase (HEPPP synthase) subunit 1 family protein

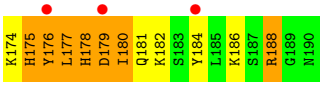


• Molecule 3: C-terminal peptide from Heptaprenyl diphosphate synthase (HEPPP synthase) subunit 1 family protein



• Molecule 3: C-terminal peptide from Heptaprenyl diphosphate synthase (HEPPP synthase) subunit 1 family protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	137.39Å 137.64Å 144.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.68 24.88 – 2.68	Depositor EDS
% Data completeness (in resolution range)	86.9 (25.00-2.68) 87.2 (24.88-2.68)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.68Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.243 , 0.287 0.243 , 0.286	Depositor DCC
R_{free} test set	1662 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	65.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8584	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.54	0/2557	0.76	1/3429 (0.0%)
1	B	0.54	0/2557	0.76	1/3429 (0.0%)
2	C	0.53	0/1579	0.77	0/2134
2	D	0.52	0/1579	0.77	0/2134
3	K	0.60	0/151	1.06	1/198 (0.5%)
3	L	0.59	0/151	1.04	1/198 (0.5%)
All	All	0.53	0/8574	0.77	4/11522 (0.0%)

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
2	D	0	1
3	K	0	1
3	L	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	GLY	N-CA-C	7.20	131.09	113.10
1	B	39	GLY	N-CA-C	7.14	130.94	113.10
3	K	177	LEU	CA-CB-CG	5.81	128.65	115.30
3	L	177	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	176	TYR	Sidechain
3	K	176	TYR	Sidechain
3	L	176	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2639	123	0
1	B	2528	0	2639	127	0
2	C	1547	0	1514	137	0
2	D	1547	0	1514	146	0
3	K	148	0	147	29	0
3	L	148	0	147	39	0
4	A	10	0	0	1	0
4	B	5	0	0	0	0
4	K	5	0	0	0	0
5	A	21	0	0	1	0
5	B	26	0	0	2	0
5	C	20	0	0	0	0
5	D	19	0	0	0	0
5	K	17	0	0	0	0
5	L	15	0	0	7	0
All	All	8584	0	8600	569	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 33.

All (569) 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:B:219:LYS:HA	1:B:219:LYS:HE3	1.27	1.13
1:A:219:LYS:HE3	1:A:219:LYS:HA	1.26	1.12
1:A:192:ARG:HB3	1:A:192:ARG:HH11	1.24	1.02
2:C:56:ARG:HG3	2:C:167:LYS:HE3	1.41	0.98
1:B:192:ARG:HH11	1:B:192:ARG:HB3	1.27	0.96
2:D:121:ILE:HG21	2:D:180:ILE:HD12	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:ILE:HG21	2:C:180:ILE:HD12	1.45	0.96
2:D:56:ARG:HG3	2:D:167:LYS:HE3	1.44	0.96
1:A:40:GLY:H	1:A:42:ARG:HH12	1.12	0.94
1:A:223:LYS:HE3	1:A:224:PRO:HD3	1.50	0.93
1:B:223:LYS:HE3	1:B:224:PRO:HD3	1.47	0.93
1:B:40:GLY:H	1:B:42:ARG:HH12	1.15	0.93
2:C:97:ILE:HG12	2:C:135:ILE:HD11	1.57	0.87
2:D:152:TYR:O	2:D:155:GLU:HB2	1.75	0.86
2:C:152:TYR:O	2:C:155:GLU:HB2	1.74	0.86
2:D:17:LYS:O	2:D:19:VAL:N	2.08	0.85
3:K:188:ARG:HB3	3:K:188:ARG:HH11	1.41	0.85
2:C:17:LYS:O	2:C:19:VAL:N	2.08	0.85
1:A:288:LEU:HD11	1:A:315:GLY:HA3	1.59	0.84
2:D:166:LYS:HB2	2:D:169:ASN:HB2	1.59	0.84
1:B:288:LEU:HD11	1:B:315:GLY:HA3	1.59	0.84
2:C:85:LEU:HD13	2:C:94:GLN:HG3	1.58	0.84
2:C:166:LYS:HB2	2:C:169:ASN:HB2	1.60	0.84
3:L:178:HIS:O	3:L:181:GLN:HG2	1.78	0.84
2:D:85:LEU:HD13	2:D:94:GLN:HG3	1.58	0.83
2:C:149:ILE:HG13	2:C:152:TYR:HB3	1.60	0.82
3:K:178:HIS:O	3:K:181:GLN:HG2	1.78	0.82
2:D:149:ILE:HG13	2:D:152:TYR:HB3	1.61	0.82
2:D:97:ILE:HG12	2:D:135:ILE:HD11	1.60	0.81
2:C:4:THR:HG21	2:C:45:LYS:HB3	1.62	0.81
2:C:182:LYS:HG2	2:C:186:LYS:HE2	1.63	0.81
2:D:59:ASP:HB3	2:D:167:LYS:HG3	1.63	0.81
2:C:40:ILE:HG22	2:C:140:PHE:HB2	1.63	0.80
1:A:214:PHE:HZ	1:A:238:ILE:HD11	1.46	0.80
2:D:161:TYR:O	2:D:163:SER:N	2.15	0.80
3:L:188:ARG:HH11	3:L:188:ARG:HB3	1.45	0.80
2:C:161:TYR:O	2:C:163:SER:N	2.13	0.80
2:C:104:ILE:HD12	2:C:128:ILE:HA	1.62	0.79
2:D:11:GLN:O	2:D:14:GLU:HG3	1.82	0.79
2:D:104:ILE:HD12	2:D:128:ILE:HA	1.64	0.79
2:C:11:GLN:O	2:C:14:GLU:HG3	1.82	0.79
1:B:283:VAL:HG13	3:L:176:TYR:CE2	2.18	0.79
2:C:59:ASP:HB3	2:C:167:LYS:HG3	1.64	0.78
2:D:4:THR:HG21	2:D:45:LYS:HB3	1.64	0.78
2:D:40:ILE:HG22	2:D:140:PHE:HB2	1.65	0.78
2:C:165:PHE:CD1	2:C:177:LEU:HD23	2.18	0.78
1:A:290:LYS:HE2	3:K:174:LYS:HD3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:LEU:HD12	2:C:137:LEU:HD11	1.64	0.78
1:B:214:PHE:HZ	1:B:238:ILE:HD11	1.46	0.77
1:B:192:ARG:HB3	1:B:192:ARG:NH1	1.99	0.77
1:B:179:VAL:O	1:B:183:THR:HG23	1.85	0.77
2:D:165:PHE:CD1	2:D:177:LEU:HD23	2.18	0.77
1:A:192:ARG:HB3	1:A:192:ARG:NH1	1.99	0.77
2:D:182:LYS:HG2	2:D:186:LYS:HE2	1.65	0.77
1:B:283:VAL:HG13	3:L:176:TYR:CZ	2.20	0.76
1:B:288:LEU:CD1	1:B:315:GLY:HA3	2.16	0.76
1:A:283:VAL:HG13	3:K:176:TYR:CE2	2.21	0.75
2:D:35:LEU:HD12	2:D:137:LEU:HD11	1.68	0.75
1:B:290:LYS:HE2	3:L:174:LYS:HD3	1.66	0.75
1:A:288:LEU:CD1	1:A:315:GLY:HA3	2.16	0.74
3:L:174:LYS:HB3	3:L:177:LEU:HB2	1.70	0.74
3:K:174:LYS:HZ1	3:K:177:LEU:HA	1.53	0.74
2:C:33:LYS:O	2:C:35:LEU:N	2.20	0.74
1:A:283:VAL:HG13	3:K:176:TYR:CZ	2.23	0.73
3:L:174:LYS:HZ1	3:L:177:LEU:HA	1.53	0.73
2:C:182:LYS:HG2	2:C:186:LYS:CE	2.17	0.73
2:C:131:LEU:O	2:C:135:ILE:HG23	1.89	0.73
2:D:33:LYS:O	2:D:35:LEU:N	2.21	0.73
2:D:27:ILE:O	2:D:27:ILE:HG22	1.89	0.73
2:C:175:HIS:H	2:C:175:HIS:CD2	2.06	0.73
3:K:174:LYS:HB3	3:K:177:LEU:HB2	1.71	0.72
1:A:317:ARG:HG2	1:A:318:ASN:H	1.54	0.72
2:C:27:ILE:HG22	2:C:27:ILE:O	1.89	0.72
2:D:175:HIS:CD2	2:D:175:HIS:H	2.07	0.72
2:D:131:LEU:O	2:D:135:ILE:HG23	1.91	0.71
1:A:64:THR:HG22	1:A:183:THR:OG1	1.90	0.71
2:C:83:THR:O	2:C:86:ALA:HB3	1.90	0.71
2:D:153:LEU:HD23	2:D:153:LEU:O	1.90	0.71
2:D:83:THR:O	2:D:86:ALA:HB3	1.91	0.71
2:D:34:LEU:HD13	2:D:156:ASP:OD2	1.91	0.70
2:C:161:TYR:CD1	2:C:162:PRO:HD2	2.26	0.70
2:C:153:LEU:HD23	2:C:153:LEU:O	1.90	0.70
1:A:179:VAL:O	1:A:183:THR:HG23	1.91	0.70
2:D:10:ARG:O	2:D:13:GLU:HB2	1.91	0.70
1:B:317:ARG:HG2	1:B:318:ASN:H	1.55	0.70
2:C:165:PHE:HD1	2:C:177:LEU:HD23	1.56	0.70
2:C:10:ARG:O	2:C:13:GLU:HB2	1.92	0.70
2:C:149:ILE:HG13	2:C:152:TYR:CB	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:GLU:HA	2:D:149:ILE:HG22	1.74	0.69
2:D:182:LYS:HG2	2:D:186:LYS:CE	2.22	0.69
2:D:51:ILE:HB	2:D:81:PHE:CD1	2.26	0.69
2:D:149:ILE:HG13	2:D:152:TYR:CB	2.22	0.69
1:A:21:ILE:HG13	1:A:32:SER:HB3	1.74	0.69
1:A:125:LYS:HD3	1:A:125:LYS:N	2.07	0.69
2:C:51:ILE:HB	2:C:81:PHE:CD1	2.26	0.69
1:B:271:ILE:O	1:B:274:SER:HB3	1.91	0.69
2:D:161:TYR:CD1	2:D:162:PRO:HD2	2.27	0.69
1:B:125:LYS:HD3	1:B:125:LYS:N	2.08	0.69
2:C:146:GLU:HA	2:C:149:ILE:HG22	1.74	0.69
2:C:34:LEU:HD13	2:C:156:ASP:OD2	1.93	0.68
3:L:174:LYS:NZ	3:L:177:LEU:HA	2.08	0.68
1:A:122:MET:CE	2:C:95:ASN:HB2	2.23	0.68
2:D:34:LEU:HD13	2:D:156:ASP:OD1	1.94	0.68
2:C:56:ARG:HG3	2:C:167:LYS:CE	2.21	0.68
3:K:174:LYS:NZ	3:K:177:LEU:HA	2.08	0.68
3:K:188:ARG:HB3	3:K:188:ARG:NH1	2.09	0.68
2:D:34:LEU:HD13	2:D:156:ASP:CG	2.14	0.67
1:B:122:MET:CE	2:D:95:ASN:HB2	2.24	0.67
2:D:165:PHE:HD1	2:D:177:LEU:HD23	1.58	0.67
2:D:56:ARG:HG3	2:D:167:LYS:CE	2.24	0.67
1:A:271:ILE:O	1:A:274:SER:HB3	1.94	0.67
3:L:174:LYS:HE3	3:L:177:LEU:HD13	1.77	0.67
1:A:219:LYS:HA	1:A:219:LYS:CE	2.11	0.66
1:B:64:THR:HG22	1:B:183:THR:OG1	1.94	0.66
1:A:159:ILE:HG12	3:K:179:ASP:OD1	1.97	0.65
1:A:288:LEU:HD11	1:A:315:GLY:CA	2.25	0.65
2:C:34:LEU:HD13	2:C:156:ASP:CG	2.17	0.65
1:B:16:ARG:HB3	1:B:69:VAL:HG21	1.76	0.65
1:B:288:LEU:HD11	1:B:315:GLY:CA	2.25	0.65
2:C:34:LEU:HD13	2:C:156:ASP:OD1	1.97	0.65
1:B:223:LYS:CE	1:B:224:PRO:HD3	2.25	0.65
1:B:219:LYS:HA	1:B:219:LYS:CE	2.13	0.64
1:A:154:SER:HB3	1:A:252:ILE:HG22	1.78	0.64
1:A:214:PHE:CZ	1:A:238:ILE:HD11	2.32	0.64
2:D:91:LEU:C	2:D:91:LEU:HD23	2.18	0.64
1:A:317:ARG:HG2	1:A:318:ASN:N	2.12	0.64
3:L:188:ARG:HB3	3:L:188:ARG:NH1	2.12	0.64
1:B:21:ILE:HG13	1:B:32:SER:HB3	1.79	0.64
1:B:157:THR:CG2	1:B:159:ILE:HG22	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:TYR:O	2:D:40:ILE:N	2.31	0.63
1:B:134:SER:O	1:B:138:VAL:HG23	1.98	0.63
2:C:38:TYR:O	2:C:40:ILE:N	2.31	0.63
3:L:177:LEU:HD11	5:L:204:HOH:O	1.98	0.63
1:A:134:SER:O	1:A:138:VAL:HG23	1.98	0.63
1:B:135:GLU:OE2	2:D:15:ARG:NH2	2.29	0.63
1:A:16:ARG:HB3	1:A:69:VAL:HG21	1.79	0.63
3:K:174:LYS:HE3	3:K:177:LEU:HD13	1.81	0.63
2:C:182:LYS:HG2	2:C:186:LYS:NZ	2.13	0.63
1:B:159:ILE:HG12	3:L:179:ASP:OD1	1.99	0.62
2:C:166:LYS:HG2	2:C:169:ASN:OD1	1.99	0.62
1:B:317:ARG:HG2	1:B:318:ASN:N	2.14	0.62
1:B:44:ARG:NH2	5:B:501:HOH:O	2.32	0.62
1:B:154:SER:HB3	1:B:252:ILE:HG22	1.81	0.62
2:C:59:ASP:CB	2:C:167:LYS:HE2	2.29	0.62
2:C:183:SER:O	2:C:184:TYR:HD1	1.82	0.62
1:A:223:LYS:CE	1:A:224:PRO:HD3	2.26	0.62
2:C:173:VAL:H	2:C:176:TYR:HD2	1.47	0.62
2:D:183:SER:O	2:D:184:TYR:HD1	1.82	0.62
1:A:157:THR:CG2	1:A:159:ILE:HG22	2.30	0.62
2:D:173:VAL:HG12	2:D:176:TYR:CD2	2.35	0.62
1:B:223:LYS:HE3	1:B:224:PRO:CD	2.26	0.61
2:D:36:ASP:C	2:D:38:TYR:H	2.03	0.61
1:A:223:LYS:HE3	1:A:224:PRO:CD	2.27	0.61
2:D:166:LYS:HG2	2:D:169:ASN:OD1	2.00	0.61
1:B:214:PHE:CZ	1:B:238:ILE:HD11	2.33	0.61
3:L:177:LEU:CD1	5:L:204:HOH:O	2.49	0.61
2:C:91:LEU:C	2:C:91:LEU:HD23	2.20	0.61
2:C:85:LEU:CD1	2:C:94:GLN:HG3	2.31	0.61
2:C:36:ASP:C	2:C:38:TYR:H	2.04	0.60
2:C:59:ASP:HB2	2:C:167:LYS:HE2	1.83	0.60
2:C:173:VAL:HG12	2:C:176:TYR:CD2	2.36	0.60
1:B:283:VAL:CG1	3:L:176:TYR:OH	2.49	0.60
1:B:291:ALA:O	1:B:295:ILE:HG13	2.02	0.60
2:C:155:GLU:OE2	2:C:188:ARG:CZ	2.50	0.60
2:D:173:VAL:H	2:D:176:TYR:HD2	1.49	0.60
1:A:178:GLU:OE1	1:A:195:LYS:HG3	2.01	0.59
2:D:59:ASP:CB	2:D:167:LYS:HE2	2.32	0.59
1:A:131:GLN:HG3	1:A:132:LEU:N	2.18	0.59
1:B:225:VAL:C	1:B:227:SER:H	2.04	0.59
1:A:316:SER:OG	1:B:257:ARG:NE	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:GLU:OE2	2:D:188:ARG:CZ	2.50	0.59
1:A:40:GLY:H	1:A:42:ARG:NH1	1.94	0.59
2:D:40:ILE:HG22	2:D:140:PHE:CB	2.31	0.59
2:D:58:LEU:HA	2:D:61:ILE:HD12	1.85	0.59
2:C:40:ILE:HG22	2:C:140:PHE:CB	2.30	0.59
2:C:56:ARG:CG	2:C:167:LYS:HE3	2.26	0.59
2:D:23:GLU:HG2	2:D:66:LEU:HD22	1.83	0.59
1:A:60:THR:HG22	1:A:64:THR:OG1	2.03	0.58
2:C:6:SER:HA	2:C:9:GLU:OE1	2.03	0.58
2:D:182:LYS:HG2	2:D:186:LYS:NZ	2.18	0.58
2:D:177:LEU:O	2:D:181:GLN:HG2	2.03	0.58
1:A:193:LYS:HD2	1:A:294:LEU:HD22	1.85	0.58
1:B:16:ARG:NH1	1:B:62:GLU:OE1	2.36	0.58
2:C:27:ILE:O	2:C:28:ASN:C	2.41	0.58
3:L:174:LYS:O	3:L:177:LEU:CB	2.51	0.58
2:D:85:LEU:CD1	2:D:94:GLN:HG3	2.31	0.58
3:L:174:LYS:HZ1	3:L:177:LEU:HD12	1.67	0.58
2:D:59:ASP:HB2	2:D:167:LYS:HE2	1.84	0.58
1:A:266:GLU:O	1:A:270:ILE:HG12	2.04	0.58
1:B:266:GLU:O	1:B:270:ILE:HG12	2.04	0.58
2:D:167:LYS:HG2	2:D:168:TYR:N	2.19	0.58
1:A:16:ARG:NH1	1:A:62:GLU:OE1	2.37	0.57
2:D:166:LYS:HE2	2:D:181:GLN:NE2	2.19	0.57
1:B:131:GLN:HG3	1:B:132:LEU:N	2.19	0.57
2:C:166:LYS:CD	2:C:166:LYS:H	2.17	0.57
2:D:6:SER:HA	2:D:9:GLU:OE1	2.05	0.57
2:D:27:ILE:O	2:D:28:ASN:C	2.43	0.57
1:B:187:ASP:N	1:B:187:ASP:OD1	2.37	0.57
1:B:193:LYS:HD2	1:B:294:LEU:HD22	1.85	0.57
2:D:56:ARG:CG	2:D:167:LYS:HE3	2.29	0.57
1:A:219:LYS:HE3	1:A:219:LYS:CA	2.17	0.57
2:C:177:LEU:O	2:C:181:GLN:HG2	2.03	0.57
2:C:188:ARG:HD3	2:C:189:GLY:N	2.19	0.57
1:A:283:VAL:CG1	3:K:176:TYR:OH	2.52	0.57
2:C:167:LYS:HG2	2:C:168:TYR:N	2.20	0.57
1:A:225:VAL:C	1:A:227:SER:H	2.05	0.57
1:B:60:THR:HG22	1:B:64:THR:OG1	2.05	0.57
2:C:58:LEU:HA	2:C:61:ILE:HD12	1.87	0.56
1:A:100:LYS:HE2	4:A:502:PO4:O3	2.05	0.56
1:B:219:LYS:HE3	1:B:219:LYS:CA	2.19	0.56
2:C:175:HIS:H	2:C:175:HIS:HD2	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:CG1	1:B:32:SER:HB3	2.36	0.56
1:B:178:GLU:OE1	1:B:195:LYS:HG3	2.05	0.56
1:A:21:ILE:CG1	1:A:32:SER:HB3	2.36	0.56
2:D:175:HIS:H	2:D:175:HIS:HD2	1.53	0.56
2:D:40:ILE:CG2	2:D:140:PHE:HB2	2.36	0.56
2:D:166:LYS:H	2:D:166:LYS:CD	2.18	0.56
1:A:187:ASP:OD1	1:A:187:ASP:N	2.39	0.56
2:C:185:LEU:HD23	2:C:185:LEU:O	2.06	0.56
1:B:157:THR:HG22	1:B:160:ASN:HB2	1.88	0.56
1:A:157:THR:HG22	1:A:160:ASN:HB2	1.88	0.56
2:C:167:LYS:NZ	2:C:168:TYR:HD1	2.03	0.56
2:D:135:ILE:HD12	2:D:135:ILE:O	2.06	0.56
2:C:16:LEU:O	2:C:17:LYS:O	2.24	0.56
2:D:167:LYS:NZ	2:D:168:TYR:HD1	2.02	0.55
1:A:135:GLU:OE2	2:C:15:ARG:NH2	2.32	0.55
1:B:136:SER:CB	1:B:175:ILE:HD11	2.36	0.55
2:D:188:ARG:HD3	2:D:189:GLY:N	2.21	0.55
1:B:194:LEU:HD23	1:B:197:ILE:HD12	1.88	0.55
2:C:127:LYS:O	2:C:131:LEU:HB2	2.07	0.55
2:C:166:LYS:HE2	2:C:181:GLN:NE2	2.21	0.55
3:K:188:ARG:HH11	3:K:188:ARG:CB	2.17	0.55
3:K:174:LYS:O	3:K:177:LEU:CB	2.55	0.55
3:L:174:LYS:HD2	3:L:177:LEU:N	2.21	0.55
2:D:185:LEU:O	2:D:185:LEU:HD23	2.06	0.55
2:C:166:LYS:HG3	2:C:168:TYR:CZ	2.42	0.55
1:A:192:ARG:HH11	1:A:192:ARG:CB	2.10	0.55
1:B:192:ARG:HH11	1:B:192:ARG:CB	2.11	0.54
2:C:177:LEU:O	2:C:177:LEU:HD12	2.08	0.54
2:D:174:LYS:O	2:D:175:HIS:C	2.46	0.54
1:A:21:ILE:HG13	1:A:32:SER:CB	2.36	0.54
1:B:251:LYS:HE2	1:B:266:GLU:OE1	2.07	0.54
2:C:23:GLU:HG2	2:C:66:LEU:HD22	1.87	0.54
2:D:16:LEU:O	2:D:17:LYS:O	2.26	0.54
2:D:127:LYS:O	2:D:131:LEU:HB2	2.08	0.54
1:A:51:SER:OG	1:A:177:THR:HA	2.07	0.54
2:D:162:PRO:HG2	2:D:182:LYS:HE2	1.89	0.54
2:C:15:ARG:NH1	2:C:80:HIS:ND1	2.56	0.54
1:B:125:LYS:HD3	1:B:125:LYS:H	1.72	0.54
3:K:174:LYS:HD2	3:K:177:LEU:N	2.22	0.54
3:L:174:LYS:HZ1	3:L:177:LEU:CD1	2.21	0.54
2:C:40:ILE:CG2	2:C:140:PHE:HB2	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG11	3:L:176:TYR:OH	2.08	0.53
2:C:174:LYS:O	2:C:175:HIS:C	2.47	0.53
2:D:166:LYS:HG3	2:D:168:TYR:CZ	2.43	0.53
1:B:5:ASN:O	1:B:9:GLU:HG2	2.09	0.53
2:C:135:ILE:O	2:C:135:ILE:HD12	2.08	0.53
2:C:162:PRO:HG2	2:C:182:LYS:HE2	1.91	0.53
2:C:166:LYS:HD2	2:C:166:LYS:N	2.22	0.53
2:C:132:PHE:O	2:C:136:THR:OG1	2.25	0.53
2:C:153:LEU:HD23	2:C:153:LEU:C	2.29	0.53
2:D:166:LYS:HD2	2:D:166:LYS:N	2.23	0.53
1:A:291:ALA:O	1:A:295:ILE:HG13	2.08	0.53
2:D:88:ILE:O	2:D:90:ASP:N	2.40	0.53
2:C:150:TYR:C	2:C:150:TYR:CD2	2.82	0.53
2:D:150:TYR:C	2:D:150:TYR:CD2	2.81	0.53
1:B:51:SER:OG	1:B:177:THR:HA	2.07	0.53
2:C:150:TYR:C	2:C:150:TYR:HD2	2.12	0.53
1:A:125:LYS:HD3	1:A:125:LYS:H	1.70	0.53
1:B:21:ILE:HG13	1:B:32:SER:CB	2.39	0.53
2:D:15:ARG:NH1	2:D:80:HIS:ND1	2.57	0.52
2:D:166:LYS:O	2:D:167:LYS:CB	2.57	0.52
1:B:300:ASP:HA	1:B:304:LYS:HD3	1.91	0.52
2:D:12:ILE:HD12	2:D:77:ILE:HG12	1.91	0.52
2:D:150:TYR:C	2:D:150:TYR:HD2	2.12	0.52
1:A:205:PHE:CD1	1:A:317:ARG:NH2	2.78	0.52
1:B:86:ASP:HB2	1:B:88:SER:OG	2.09	0.52
2:D:166:LYS:H	2:D:166:LYS:HD2	1.75	0.52
2:D:153:LEU:HD23	2:D:153:LEU:C	2.29	0.52
2:D:177:LEU:O	2:D:177:LEU:HD12	2.09	0.51
1:A:318:ASN:O	1:A:319:THR:HB	2.10	0.51
1:A:136:SER:CB	1:A:175:ILE:HD11	2.40	0.51
1:A:5:ASN:O	1:A:9:GLU:HG2	2.10	0.51
2:C:88:ILE:O	2:C:90:ASP:N	2.41	0.51
2:C:166:LYS:O	2:C:167:LYS:CB	2.57	0.51
2:D:189:GLY:O	2:D:190:ASN:HB2	2.11	0.51
1:A:154:SER:OG	1:A:253:GLU:HA	2.11	0.51
2:D:91:LEU:HD23	2:D:91:LEU:O	2.11	0.51
3:L:177:LEU:CD2	5:L:204:HOH:O	2.59	0.51
3:L:177:LEU:HD21	5:L:204:HOH:O	2.10	0.51
1:B:317:ARG:HD3	1:B:319:THR:OXT	2.11	0.51
2:D:68:LYS:N	2:D:68:LYS:CD	2.74	0.51
2:D:166:LYS:O	2:D:167:LYS:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:LEU:HD23	2:C:91:LEU:O	2.11	0.51
1:A:86:ASP:HB2	1:A:88:SER:OG	2.11	0.51
1:A:147:GLN:OE1	1:A:168:LYS:HD2	2.11	0.50
1:B:205:PHE:CD1	1:B:317:ARG:NH2	2.77	0.50
3:L:174:LYS:O	3:L:177:LEU:HB2	2.11	0.50
1:A:41:LYS:HG3	1:A:43:VAL:HG12	1.94	0.50
2:C:166:LYS:O	2:C:167:LYS:HB3	2.12	0.50
2:D:119:TYR:O	2:D:123:GLN:HG2	2.12	0.50
3:K:174:LYS:HZ1	3:K:177:LEU:HD12	1.76	0.50
3:L:174:LYS:CE	3:L:177:LEU:HD13	2.42	0.50
1:A:197:ILE:HD13	1:A:295:ILE:HG12	1.93	0.50
1:B:157:THR:HG21	1:B:159:ILE:HG22	1.93	0.50
2:C:173:VAL:N	2:C:176:TYR:HD2	2.09	0.50
1:A:132:LEU:HD23	1:A:132:LEU:C	2.32	0.50
1:A:256:ARG:NH1	1:A:258:ASP:OD2	2.45	0.50
1:B:286:LYS:NZ	3:L:175:HIS:CE1	2.80	0.50
1:B:318:ASN:O	1:B:319:THR:HB	2.12	0.50
1:A:283:VAL:HG11	3:K:176:TYR:OH	2.11	0.50
2:C:93:PHE:O	2:C:97:ILE:HB	2.11	0.50
3:L:186:LYS:NZ	5:L:201:HOH:O	2.45	0.50
1:B:156:GLN:NE2	1:B:164:ARG:HH12	2.10	0.49
2:C:68:LYS:N	2:C:68:LYS:CD	2.75	0.49
2:D:59:ASP:OD2	2:D:167:LYS:HE2	2.12	0.49
3:L:188:ARG:HH11	3:L:188:ARG:CB	2.20	0.49
2:C:189:GLY:O	2:C:190:ASN:HB2	2.12	0.49
1:A:317:ARG:HD3	1:A:319:THR:OXT	2.12	0.49
2:C:59:ASP:OD2	2:C:167:LYS:HE2	2.13	0.49
2:C:166:LYS:H	2:C:166:LYS:HD2	1.75	0.49
1:A:251:LYS:HE2	1:A:266:GLU:OE1	2.13	0.49
1:B:132:LEU:C	1:B:132:LEU:HD23	2.33	0.49
2:C:4:THR:CG2	2:C:45:LYS:HD3	2.42	0.49
2:D:93:PHE:O	2:D:97:ILE:HB	2.13	0.49
2:D:4:THR:CG2	2:D:45:LYS:HD3	2.42	0.49
1:B:44:ARG:O	1:B:48:VAL:HG23	2.13	0.49
1:B:154:SER:OG	1:B:253:GLU:HA	2.13	0.49
2:C:165:PHE:HA	2:C:177:LEU:HD21	1.95	0.49
2:D:183:SER:O	2:D:184:TYR:CD1	2.65	0.49
1:B:256:ARG:NH1	1:B:258:ASP:OD2	2.46	0.49
1:B:41:LYS:HG3	1:B:43:VAL:HG12	1.95	0.48
2:C:155:GLU:CG	2:C:188:ARG:NH2	2.76	0.48
1:A:225:VAL:C	1:A:227:SER:N	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:TYR:O	2:C:123:GLN:HG2	2.14	0.48
2:D:155:GLU:CG	2:D:188:ARG:NH2	2.76	0.48
1:A:286:LYS:NZ	3:K:175:HIS:CE1	2.81	0.48
3:K:181:GLN:HA	3:K:184:TYR:CD1	2.49	0.48
1:B:147:GLN:OE1	1:B:168:LYS:HD2	2.14	0.48
1:B:286:LYS:HD2	3:L:176:TYR:HD2	1.78	0.48
2:D:36:ASP:C	2:D:38:TYR:N	2.66	0.48
1:B:283:VAL:HG13	3:L:176:TYR:OH	2.14	0.48
2:D:173:VAL:N	2:D:176:TYR:HD2	2.10	0.48
1:A:265:GLU:O	1:A:269:GLN:HB2	2.14	0.48
2:C:153:LEU:C	2:C:155:GLU:H	2.17	0.48
2:D:132:PHE:O	2:D:136:THR:OG1	2.26	0.48
2:C:33:LYS:O	2:C:34:LEU:C	2.52	0.48
2:C:47:ALA:HA	2:C:84:LEU:HD23	1.96	0.48
2:D:78:SER:O	2:D:81:PHE:HB3	2.14	0.48
1:A:157:THR:HG23	1:A:159:ILE:HG22	1.95	0.48
1:A:241:GLU:OE2	1:A:241:GLU:HA	2.13	0.48
2:C:51:ILE:HB	2:C:81:PHE:CE1	2.49	0.47
3:L:181:GLN:HA	3:L:184:TYR:CD1	2.49	0.47
1:B:193:LYS:O	1:B:197:ILE:HG13	2.14	0.47
2:C:183:SER:O	2:C:184:TYR:CD1	2.65	0.47
2:D:51:ILE:HB	2:D:81:PHE:CE1	2.48	0.47
2:D:122:SER:OG	2:D:184:TYR:CG	2.67	0.47
1:A:152:PHE:CD1	1:A:256:ARG:HA	2.49	0.47
2:D:174:LYS:C	2:D:178:HIS:HD1	2.14	0.47
1:A:100:LYS:HB3	1:A:101:TRP:CE3	2.49	0.47
1:A:300:ASP:HA	1:A:304:LYS:HD3	1.96	0.47
2:C:182:LYS:O	2:C:186:LYS:HE2	2.14	0.47
1:A:223:LYS:HG3	1:A:224:PRO:HD2	1.97	0.47
1:B:265:GLU:O	1:B:269:GLN:HB2	2.14	0.47
1:A:67:VAL:O	1:A:71:LEU:HD23	2.15	0.47
1:A:132:LEU:HD11	1:A:178:GLU:OE2	2.14	0.47
2:D:153:LEU:C	2:D:155:GLU:H	2.18	0.47
3:K:174:LYS:O	3:K:177:LEU:HB2	2.14	0.47
1:A:44:ARG:NH2	5:A:601:HOH:O	2.47	0.47
1:A:285:SER:OG	1:B:258:ASP:HB2	2.15	0.47
1:A:156:GLN:NE2	1:A:164:ARG:HH12	2.13	0.47
2:C:146:GLU:CA	2:C:149:ILE:HG22	2.43	0.47
2:D:47:ALA:HA	2:D:84:LEU:HD23	1.97	0.47
3:L:186:LYS:HE3	5:L:201:HOH:O	2.15	0.47
1:A:91:ARG:HB2	1:A:96:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:HG2	1:A:224:PRO:HA	1.97	0.46
1:B:197:ILE:HD13	1:B:295:ILE:HG12	1.96	0.46
1:B:304:LYS:O	1:B:308:LEU:HD12	2.15	0.46
1:B:241:GLU:HA	1:B:241:GLU:OE2	2.13	0.46
1:A:304:LYS:O	1:A:308:LEU:HD12	2.15	0.46
2:C:36:ASP:C	2:C:38:TYR:N	2.67	0.46
2:C:175:HIS:O	2:C:176:TYR:C	2.53	0.46
2:D:33:LYS:O	2:D:34:LEU:C	2.53	0.46
2:D:182:LYS:O	2:D:186:LYS:HE2	2.15	0.46
1:B:223:LYS:HG3	1:B:224:PRO:HD2	1.97	0.46
2:C:149:ILE:CG1	2:C:152:TYR:HB3	2.39	0.46
2:C:151:ASN:OD1	2:C:188:ARG:CG	2.63	0.46
2:C:173:VAL:O	2:C:176:TYR:HB2	2.15	0.46
1:B:225:VAL:C	1:B:227:SER:N	2.64	0.46
1:B:283:VAL:CG1	3:L:176:TYR:CZ	2.94	0.46
2:C:174:LYS:C	2:C:178:HIS:HD1	2.14	0.46
1:A:182:ILE:HG22	1:A:182:ILE:O	2.15	0.46
2:C:4:THR:CG2	2:C:45:LYS:HB3	2.41	0.46
1:A:194:LEU:HD23	1:A:197:ILE:HD12	1.96	0.46
1:A:199:HIS:HE1	3:K:180:ILE:HD12	1.81	0.46
1:B:16:ARG:HB3	1:B:69:VAL:CG2	2.46	0.46
1:B:157:THR:HG23	1:B:159:ILE:HG22	1.96	0.46
2:D:146:GLU:CA	2:D:149:ILE:HG22	2.43	0.46
2:D:165:PHE:HA	2:D:177:LEU:HD21	1.97	0.46
2:D:175:HIS:O	2:D:176:TYR:C	2.53	0.46
1:A:136:SER:O	1:A:140:VAL:HG23	2.16	0.46
1:A:286:LYS:HD2	3:K:176:TYR:HD2	1.80	0.46
2:D:173:VAL:O	2:D:176:TYR:HB2	2.15	0.46
1:A:4:LEU:HD22	1:A:53:GLN:CD	2.37	0.46
1:A:157:THR:HG21	1:A:159:ILE:HG22	1.97	0.46
2:C:78:SER:O	2:C:81:PHE:HB3	2.16	0.46
2:D:151:ASN:OD1	2:D:188:ARG:CG	2.63	0.45
2:C:167:LYS:HG2	2:C:168:TYR:H	1.80	0.45
2:D:68:LYS:O	2:D:71:ILE:HG13	2.16	0.45
3:L:180:ILE:O	3:L:180:ILE:HG22	2.16	0.45
1:A:222:GLY:O	1:A:223:LYS:HD2	2.17	0.45
1:B:199:HIS:HE1	3:L:180:ILE:HD12	1.80	0.45
1:B:218:GLU:HG2	1:B:224:PRO:HA	1.98	0.45
2:C:68:LYS:O	2:C:71:ILE:HG13	2.17	0.45
2:C:170:GLN:HG2	2:C:171:SER:N	2.32	0.45
2:D:46:VAL:O	2:D:50:THR:OG1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:HIS:O	2:D:182:LYS:HB2	2.17	0.45
1:B:91:ARG:HB2	1:B:96:THR:HG22	1.98	0.45
1:B:100:LYS:HB3	1:B:101:TRP:CE3	2.51	0.45
2:D:27:ILE:O	2:D:27:ILE:CG2	2.59	0.45
2:D:167:LYS:HG2	2:D:168:TYR:H	1.80	0.45
2:D:175:HIS:CD2	2:D:175:HIS:N	2.83	0.45
3:K:180:ILE:HG22	3:K:180:ILE:O	2.16	0.45
1:A:136:SER:HB3	1:A:175:ILE:HD11	1.99	0.45
1:B:222:GLY:O	1:B:223:LYS:HD2	2.17	0.45
2:C:122:SER:OG	2:C:184:TYR:CG	2.67	0.45
2:C:166:LYS:HE2	2:C:181:GLN:HE22	1.81	0.45
2:C:33:LYS:HB3	2:C:34:LEU:H	1.50	0.45
3:K:174:LYS:O	3:K:177:LEU:N	2.43	0.45
1:B:100:LYS:HD3	1:B:101:TRP:CZ3	2.52	0.44
3:L:174:LYS:O	3:L:177:LEU:N	2.40	0.44
1:B:89:ASP:OD2	1:B:89:ASP:N	2.49	0.44
1:B:152:PHE:CD1	1:B:256:ARG:HA	2.52	0.44
2:C:37:SER:O	2:C:39:ASP:N	2.51	0.44
2:D:151:ASN:OD1	2:D:188:ARG:HG3	2.17	0.44
3:K:174:LYS:HZ1	3:K:177:LEU:CD1	2.31	0.44
1:B:41:LYS:HG3	1:B:43:VAL:CG1	2.48	0.44
2:C:151:ASN:OD1	2:C:188:ARG:HG3	2.17	0.44
2:D:166:LYS:HE2	2:D:181:GLN:HE22	1.80	0.44
1:A:157:THR:HG23	1:A:160:ASN:H	1.83	0.44
1:A:226:GLY:O	1:A:229:LEU:N	2.50	0.44
1:B:4:LEU:HD22	1:B:53:GLN:CD	2.38	0.44
2:D:11:GLN:HB3	2:D:80:HIS:NE2	2.33	0.44
1:B:132:LEU:HD11	1:B:178:GLU:OE2	2.16	0.44
1:A:272:ARG:C	1:A:274:SER:H	2.21	0.44
1:B:122:MET:HE1	2:D:95:ASN:HB2	1.97	0.44
1:B:216:SER:HB3	1:B:221:LEU:HG	2.00	0.44
1:A:41:LYS:HG3	1:A:43:VAL:CG1	2.48	0.44
2:C:153:LEU:C	2:C:155:GLU:N	2.71	0.44
1:B:24:LYS:NZ	5:B:502:HOH:O	2.51	0.44
2:D:153:LEU:C	2:D:155:GLU:N	2.72	0.44
1:A:273:LYS:HG3	1:A:273:LYS:O	2.17	0.43
1:B:67:VAL:HG11	1:B:179:VAL:CG1	2.48	0.43
2:C:178:HIS:O	2:C:182:LYS:HB2	2.18	0.43
2:D:31:LEU:HD11	2:D:133:PRO:HB3	2.00	0.43
2:D:104:ILE:CD1	2:D:128:ILE:HA	2.41	0.43
1:B:226:GLY:O	1:B:229:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LYS:O	1:B:314:MET:C	2.56	0.43
2:C:151:ASN:OD1	2:C:188:ARG:HB2	2.18	0.43
2:D:144:ILE:O	2:D:144:ILE:HG13	2.18	0.43
1:A:44:ARG:O	1:A:48:VAL:HG23	2.17	0.43
2:C:11:GLN:HB3	2:C:80:HIS:NE2	2.34	0.43
1:B:205:PHE:HD1	1:B:317:ARG:NH2	2.16	0.43
2:C:38:TYR:O	2:C:39:ASP:C	2.56	0.43
2:C:177:LEU:HD12	2:C:177:LEU:C	2.39	0.43
2:D:151:ASN:OD1	2:D:188:ARG:HB2	2.18	0.43
1:A:264:PHE:O	1:A:268:ILE:HG23	2.19	0.43
1:A:313:LYS:O	1:A:314:MET:C	2.56	0.43
1:B:273:LYS:O	1:B:273:LYS:HG3	2.18	0.43
2:D:189:GLY:O	2:D:190:ASN:CB	2.67	0.43
1:B:40:GLY:H	1:B:42:ARG:NH1	1.98	0.43
2:C:31:LEU:HD11	2:C:133:PRO:HB3	2.01	0.43
2:C:173:VAL:HG22	2:C:174:LYS:N	2.34	0.43
2:D:170:GLN:HG2	2:D:171:SER:N	2.32	0.43
2:C:144:ILE:O	2:C:144:ILE:HG13	2.19	0.43
1:B:67:VAL:HG11	1:B:179:VAL:HG11	2.00	0.43
2:D:37:SER:O	2:D:39:ASP:N	2.51	0.43
2:D:135:ILE:HD12	2:D:135:ILE:C	2.40	0.43
1:A:100:LYS:HD3	1:A:101:TRP:CZ3	2.54	0.42
3:K:174:LYS:CE	3:K:177:LEU:HD13	2.48	0.42
1:A:224:PRO:O	1:A:225:VAL:HB	2.19	0.42
1:A:281:LYS:O	1:A:284:SER:HB3	2.19	0.42
1:B:319:THR:HG23	1:B:319:THR:O	2.18	0.42
2:C:81:PHE:CZ	2:C:85:LEU:HD21	2.54	0.42
3:L:174:LYS:O	3:L:177:LEU:HB3	2.19	0.42
1:A:86:ASP:C	1:A:88:SER:N	2.72	0.42
1:B:67:VAL:O	1:B:71:LEU:HD23	2.18	0.42
1:B:152:PHE:HE2	1:B:257:ARG:HG3	1.84	0.42
1:A:67:VAL:HG11	1:A:179:VAL:HG11	2.00	0.42
2:D:149:ILE:CG1	2:D:152:TYR:HB3	2.40	0.42
1:A:67:VAL:HG11	1:A:179:VAL:CG1	2.49	0.42
2:C:12:ILE:HD12	2:C:77:ILE:HG12	2.00	0.42
2:D:166:LYS:HD3	2:D:177:LEU:CD2	2.50	0.42
2:D:177:LEU:HD12	2:D:177:LEU:C	2.39	0.42
2:C:8:LEU:HB2	2:C:46:VAL:HG23	2.02	0.42
2:C:46:VAL:O	2:C:50:THR:OG1	2.29	0.42
1:A:36:LEU:O	1:A:42:ARG:NH2	2.52	0.42
1:B:23:SER:HB2	1:B:112:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:ILE:O	2:C:149:ILE:HG23	2.20	0.42
2:D:38:TYR:O	2:D:39:ASP:C	2.57	0.42
1:A:122:MET:O	1:A:122:MET:HG3	2.19	0.42
2:C:189:GLY:O	2:C:190:ASN:CB	2.67	0.42
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.86	0.42
1:A:187:ASP:O	1:A:188:LYS:C	2.58	0.42
2:C:88:ILE:C	2:C:90:ASP:H	2.23	0.42
2:D:88:ILE:C	2:D:90:ASP:H	2.23	0.42
1:B:240:LEU:HD13	1:B:279:GLU:HB3	2.02	0.41
1:A:216:SER:HB3	1:A:221:LEU:HG	2.01	0.41
1:B:157:THR:HG22	1:B:160:ASN:CB	2.49	0.41
1:B:187:ASP:O	1:B:188:LYS:C	2.58	0.41
1:A:283:VAL:HG13	3:K:176:TYR:OH	2.15	0.41
1:B:139:ASP:HA	1:B:142:ARG:HG2	2.01	0.41
1:B:229:LEU:HD13	1:B:238:ILE:HD13	2.01	0.41
1:B:250:LEU:O	1:B:254:GLN:HG2	2.20	0.41
1:A:85:ILE:HA	2:C:68:LYS:HB3	2.01	0.41
1:A:139:ASP:HA	1:A:142:ARG:HG2	2.02	0.41
1:B:264:PHE:O	1:B:268:ILE:HG23	2.20	0.41
1:B:281:LYS:O	1:B:284:SER:HB3	2.20	0.41
2:C:104:ILE:CD1	2:C:128:ILE:HA	2.42	0.41
3:L:186:LYS:CE	5:L:201:HOH:O	2.68	0.41
2:C:150:TYR:HD2	2:C:150:TYR:O	2.04	0.41
2:D:4:THR:CG2	2:D:45:LYS:HB3	2.42	0.41
1:B:161:TYR:CD1	1:B:161:TYR:C	2.94	0.41
2:D:141:GLY:O	2:D:142:ILE:O	2.39	0.41
2:D:173:VAL:HG22	2:D:174:LYS:N	2.35	0.41
3:L:179:ASP:HA	3:L:182:LYS:HD2	2.02	0.41
1:A:152:PHE:HE2	1:A:257:ARG:HG3	1.86	0.41
1:B:85:ILE:HA	2:D:68:LYS:HB3	2.02	0.41
1:B:272:ARG:C	1:B:274:SER:H	2.22	0.41
2:D:8:LEU:HB2	2:D:46:VAL:HG23	2.02	0.41
2:D:81:PHE:CZ	2:D:85:LEU:HD21	2.55	0.41
1:A:283:VAL:CG1	3:K:176:TYR:CZ	2.98	0.41
2:D:12:ILE:CD1	2:D:77:ILE:HG12	2.50	0.41
2:D:121:ILE:CG2	2:D:180:ILE:HD12	2.33	0.41
1:B:86:ASP:C	1:B:88:SER:N	2.72	0.41
1:B:279:GLU:O	1:B:282:ALA:HB3	2.21	0.41
2:C:15:ARG:HH12	2:C:80:HIS:CE1	2.39	0.41
2:C:46:VAL:HG13	2:C:84:LEU:HD21	2.02	0.41
2:C:90:ASP:OD1	2:C:90:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:LYS:HB3	2:D:34:LEU:H	1.49	0.41
2:D:121:ILE:O	2:D:125:ILE:HG13	2.21	0.41
2:D:166:LYS:CD	2:D:166:LYS:N	2.80	0.41
1:A:157:THR:HG22	1:A:160:ASN:CB	2.50	0.41
1:A:296:SER:C	1:A:298:LEU:H	2.25	0.41
1:B:36:LEU:O	1:B:42:ARG:NH2	2.54	0.41
2:C:167:LYS:CG	2:C:168:TYR:N	2.84	0.41
2:D:48:CYS:HB2	2:D:136:THR:HG21	2.03	0.41
2:D:150:TYR:HD2	2:D:150:TYR:O	2.04	0.41
1:B:182:ILE:O	1:B:182:ILE:HG22	2.20	0.40
2:C:141:GLY:O	2:C:142:ILE:O	2.39	0.40
1:A:89:ASP:OD2	1:A:89:ASP:N	2.50	0.40
1:A:200:TYR:CE2	1:A:290:LYS:HB3	2.56	0.40
2:D:149:ILE:O	2:D:149:ILE:HG23	2.20	0.40
2:D:155:GLU:HG3	2:D:188:ARG:NH2	2.36	0.40
1:A:16:ARG:HB3	1:A:69:VAL:CG2	2.48	0.40
1:A:182:ILE:O	1:A:182:ILE:CG2	2.69	0.40
1:A:319:THR:HG23	1:A:319:THR:O	2.21	0.40
1:B:37:SER:C	1:B:39:GLY:N	2.74	0.40
1:B:264:PHE:O	1:B:268:ILE:CG2	2.69	0.40
2:D:30:ARG:O	2:D:33:LYS:N	2.54	0.40
3:K:174:LYS:O	3:K:177:LEU:HB3	2.22	0.40
1:A:94:LYS:HB3	1:A:94:LYS:NZ	2.37	0.40
1:A:317:ARG:CG	1:A:318:ASN:N	2.84	0.40
1:B:136:SER:HB3	1:B:175:ILE:HD11	2.02	0.40
1:B:122:MET:O	1:B:122:MET:HG3	2.22	0.40
1:B:200:TYR:CD2	1:B:290:LYS:HB3	2.57	0.40
1:B:286:LYS:HZ1	3:L:175:HIS:CE1	2.40	0.40
2:D:68:LYS:C	2:D:70:SER:N	2.74	0.40
3:L:178:HIS:O	3:L:181:GLN:CG	2.61	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	316/319 (99%)	292 (92%)	19 (6%)	5 (2%)	9 22
1	B	316/319 (99%)	292 (92%)	19 (6%)	5 (2%)	9 22
2	C	186/190 (98%)	135 (73%)	29 (16%)	22 (12%)	0 0
2	D	186/190 (98%)	135 (73%)	28 (15%)	23 (12%)	0 0
3	K	15/17 (88%)	9 (60%)	3 (20%)	3 (20%)	0 0
3	L	15/17 (88%)	9 (60%)	3 (20%)	3 (20%)	0 0
All	All	1034/1052 (98%)	872 (84%)	101 (10%)	61 (6%)	1 2

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLY
1	A	224	PRO
1	A	225	VAL
1	B	39	GLY
1	B	224	PRO
1	B	225	VAL
2	C	17	LYS
2	C	18	GLY
2	C	20	SER
2	C	23	GLU
2	C	33	LYS
2	C	34	LEU
2	C	38	TYR
2	C	39	ASP
2	C	142	ILE
2	C	156	ASP
2	C	159	ASP
2	C	176	TYR
2	C	184	TYR
2	D	17	LYS
2	D	18	GLY
2	D	20	SER
2	D	23	GLU
2	D	33	LYS
2	D	34	LEU
2	D	38	TYR
2	D	39	ASP

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Mol	Chain	Res	Type
2	D	142	ILE
2	D	156	ASP
2	D	159	ASP
2	D	176	TYR
2	D	184	TYR
3	K	178	HIS
3	L	178	HIS
1	A	261	ARG
1	B	261	ARG
2	C	25	ILE
2	C	28	ASN
2	C	89	ASN
2	C	162	PRO
2	C	167	LYS
2	D	25	ILE
2	D	28	ASN
2	D	89	ASN
2	D	162	PRO
2	D	167	LYS
3	K	179	ASP
3	L	179	ASP
1	A	188	LYS
1	B	188	LYS
2	C	41	PRO
2	D	41	PRO
2	C	175	HIS
2	D	138	SER
2	D	175	HIS
2	C	138	SER
2	C	187	SER
2	D	187	SER
3	K	180	ILE
3	L	180	ILE
2	D	161	TYR

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	288/289 (100%)	262 (91%)	26 (9%)	9 20
1	B	288/289 (100%)	259 (90%)	29 (10%)	7 16
2	C	176/178 (99%)	150 (85%)	26 (15%)	3 6
2	D	176/178 (99%)	148 (84%)	28 (16%)	2 5
3	K	16/16 (100%)	14 (88%)	2 (12%)	4 9
3	L	16/16 (100%)	14 (88%)	2 (12%)	4 9
All	All	960/966 (99%)	847 (88%)	113 (12%)	5 11

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	16	ARG
1	A	21	ILE
1	A	28	LEU
1	A	44	ARG
1	A	56	LYS
1	A	91	ARG
1	A	94	LYS
1	A	98	SER
1	A	125	LYS
1	A	131	GLN
1	A	142	ARG
1	A	156	GLN
1	A	159	ILE
1	A	161	TYR
1	A	187	ASP
1	A	192	ARG
1	A	193	LYS
1	A	209	ASP
1	A	219	LYS
1	A	223	LYS
1	A	258	ASP
1	A	260	GLU
1	A	261	ARG
1	A	266	GLU
1	A	268	ILE
1	B	6	MET
1	B	16	ARG
1	B	21	ILE
1	B	28	LEU

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Mol	Chain	Res	Type
1	B	44	ARG
1	B	56	LYS
1	B	91	ARG
1	B	94	LYS
1	B	98	SER
1	B	125	LYS
1	B	131	GLN
1	B	142	ARG
1	B	156	GLN
1	B	157	THR
1	B	159	ILE
1	B	161	TYR
1	B	187	ASP
1	B	192	ARG
1	B	193	LYS
1	B	201	ILE
1	B	209	ASP
1	B	213	ASP
1	B	219	LYS
1	B	223	LYS
1	B	258	ASP
1	B	260	GLU
1	B	261	ARG
1	B	266	GLU
1	B	268	ILE
2	C	14	GLU
2	C	15	ARG
2	C	21	GLU
2	C	23	GLU
2	C	43	VAL
2	C	68	LYS
2	C	69	HIS
2	C	84	LEU
2	C	92	SER
2	C	97	ILE
2	C	99	LYS
2	C	135	ILE
2	C	148	GLU
2	C	150	TYR
2	C	151	ASN
2	C	152	TYR
2	C	156	ASP

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Mol	Chain	Res	Type
2	C	161	TYR
2	C	169	ASN
2	C	170	GLN
2	C	171	SER
2	C	172	GLU
2	C	175	HIS
2	C	180	ILE
2	C	184	TYR
2	C	188	ARG
2	D	14	GLU
2	D	15	ARG
2	D	21	GLU
2	D	23	GLU
2	D	24	SER
2	D	43	VAL
2	D	68	LYS
2	D	69	HIS
2	D	84	LEU
2	D	92	SER
2	D	97	ILE
2	D	99	LYS
2	D	135	ILE
2	D	148	GLU
2	D	150	TYR
2	D	151	ASN
2	D	152	TYR
2	D	156	ASP
2	D	161	TYR
2	D	169	ASN
2	D	170	GLN
2	D	171	SER
2	D	172	GLU
2	D	175	HIS
2	D	180	ILE
2	D	181	GLN
2	D	184	TYR
2	D	188	ARG
3	K	175	HIS
3	K	188	ARG
3	L	175	HIS
3	L	188	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	63	GLN
1	A	131	GLN
1	A	199	HIS
1	B	59	GLN
1	B	63	GLN
1	B	131	GLN
1	B	199	HIS
2	C	89	ASN
2	C	94	GLN
2	C	175	HIS
2	C	181	GLN
2	D	89	ASN
2	D	94	GLN
2	D	175	HIS
2	D	181	GLN
3	K	175	HIS
3	L	175	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	K	201	-	4,4,4	1.51	0	6,6,6	0.43	0
4	PO4	A	502	-	4,4,4	1.66	0	6,6,6	0.43	0
4	PO4	B	401	-	4,4,4	1.41	0	6,6,6	0.46	0
4	PO4	A	501	-	4,4,4	1.50	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	318/319 (99%)	0.08	5 (1%)	72	73	44, 65, 93, 111	2 (0%)
1	B	318/319 (99%)	0.11	6 (1%)	66	67	44, 65, 93, 111	2 (0%)
2	C	188/190 (98%)	0.53	14 (7%)	14	12	48, 81, 136, 147	0
2	D	188/190 (98%)	0.55	15 (7%)	12	10	49, 81, 136, 147	0
3	K	17/17 (100%)	0.76	2 (11%)	4	3	87, 96, 103, 106	0
3	L	17/17 (100%)	0.66	3 (17%)	1	1	87, 96, 104, 106	0
All	All	1046/1052 (99%)	0.27	45 (4%)	35	33	44, 70, 117, 147	4 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	147	SER	8.1
2	C	162	PRO	7.9
2	D	142	ILE	7.8
2	D	144	ILE	7.5
2	C	142	ILE	7.4
2	C	144	ILE	7.3
2	D	162	PRO	6.2
2	D	143	ASN	6.1
2	C	143	ASN	5.4
2	D	161	TYR	4.9
3	K	176	TYR	4.7
3	L	184	TYR	4.5
2	C	177	LEU	4.2
2	D	149	ILE	4.1
2	D	160	TYR	3.7
3	L	176	TYR	3.6
2	D	148	GLU	3.6
1	B	2	ALA	3.2
2	D	38	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	190	ASN	3.2
2	C	8	LEU	3.1
1	B	319	THR	3.1
1	B	273	LYS	3.1
1	B	264	PHE	2.9
3	K	184	TYR	2.9
2	C	166	LYS	2.9
1	A	319	THR	2.8
1	A	2	ALA	2.7
2	C	161	TYR	2.7
2	D	150	TYR	2.7
2	D	177	LEU	2.6
2	C	147	SER	2.6
2	D	166	LYS	2.6
1	A	318	ASN	2.5
2	C	38	TYR	2.5
1	A	49	ILE	2.4
2	D	43	VAL	2.4
1	B	125	LYS	2.3
2	C	160	TYR	2.3
2	D	146	GLU	2.2
2	C	153	LEU	2.2
1	B	318	ASN	2.1
3	L	179	ASP	2.1
1	A	221	LEU	2.0
2	C	188	ARG	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	K	201	5/5	0.86	0.15	130,130,131,132	0
4	PO4	A	502	5/5	0.90	0.16	146,146,147,147	0
4	PO4	B	401	5/5	0.91	0.15	95,96,96,98	0
4	PO4	A	501	5/5	0.91	0.14	107,107,108,109	0

6.5 Other polymers (i)

There are no such residues in this entry.