Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 04:36 PM EDT

PDB ID	:	2NXH
Title	:	Structural and mechanistic changes along an engineered path from metallo to non-metallo KDO8P synthase.
Authors	:	Kona, F.; Xu, X.; Martin, P.; Kuzmic, P.; Gatti, D.L.
Deposited on	:	2006-11-17
Resolution	:	2.11 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 (i) 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 (i)) were used in the production of this report:

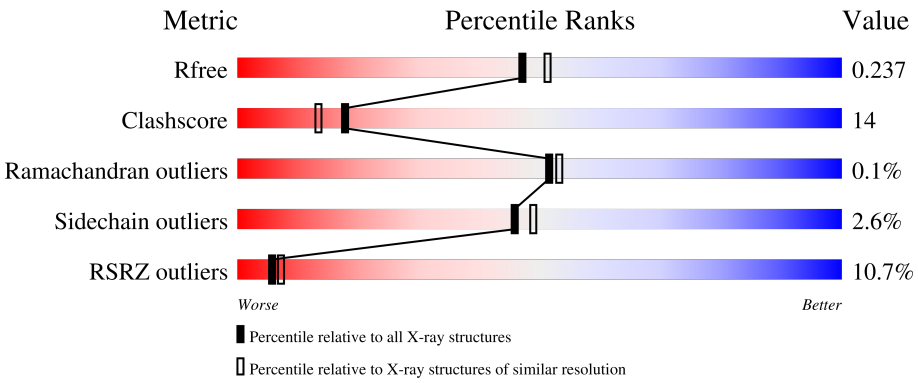
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	263	5% 79% 19% •
1	B	263	6% 78% 20% •
1	C	263	7% 73% 25% •
1	D	263	12% 69% 30% •
1	E	263	18% 65% 33% •

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Mol	Chain	Length	Quality of chain
1	F	263	27% 57% 41%
1	G	263	6% 77% 21%
1	H	263	3% 72% 24%
1	I	263	6% 78% 20%
1	J	263	3% 71% 24%
1	K	263	24% 62% 36%
1	L	263	11% 73% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26278 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-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	2056	1327	344	380	5	0	0	0
1	B	262	2056	1327	344	380	5	0	0	0
1	C	262	2056	1327	344	380	5	0	0	0
1	D	262	2056	1327	344	380	5	0	0	0
1	E	259	2035	1315	340	375	5	0	0	0
1	F	262	2056	1327	344	380	5	0	0	0
1	G	262	2056	1327	344	380	5	0	0	0
1	H	256	2017	1304	337	371	5	0	0	0
1	I	262	2056	1327	344	380	5	0	0	0
1	J	255	2013	1302	336	370	5	0	0	0
1	K	262	2056	1327	344	380	5	0	0	0
1	L	262	2056	1327	344	380	5	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1011	ASN	CYS	engineered mutation	UNP O66496
A	1235	PRO	SER	engineered mutation	UNP O66496
A	1237	ALA	GLN	engineered mutation	UNP O66496
B	2011	ASN	CYS	engineered mutation	UNP O66496
B	2235	PRO	SER	engineered mutation	UNP O66496

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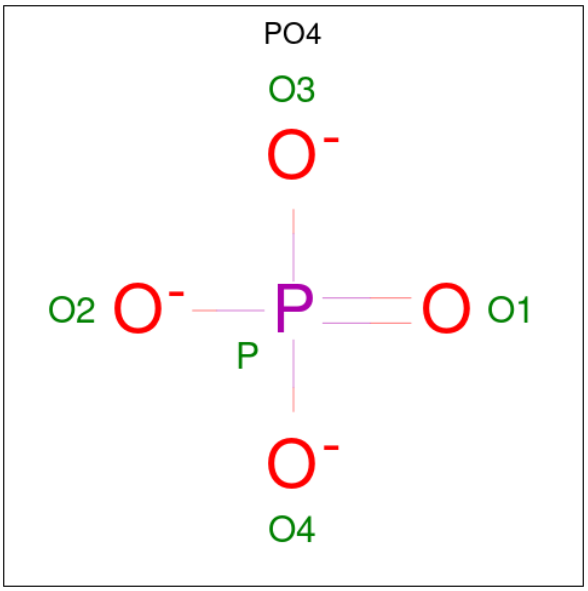
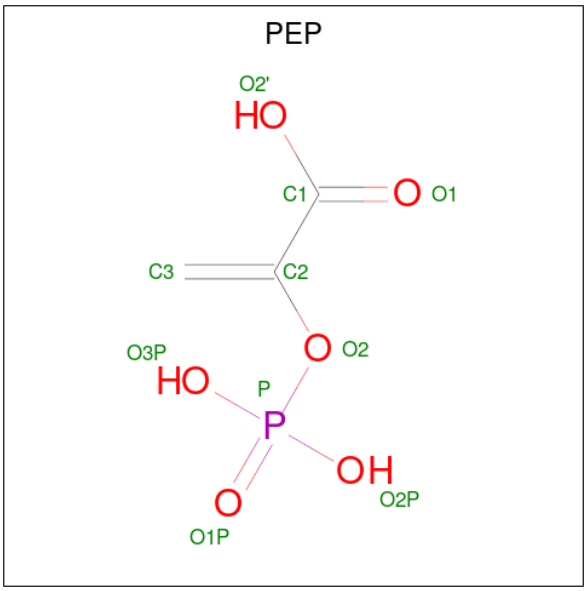
Chain	Residue	Modelled	Actual	Comment	Reference
B	2237	ALA	GLN	engineered mutation	UNP O66496
C	3011	ASN	CYS	engineered mutation	UNP O66496
C	3235	PRO	SER	engineered mutation	UNP O66496
C	3237	ALA	GLN	engineered mutation	UNP O66496
D	4011	ASN	CYS	engineered mutation	UNP O66496
D	4235	PRO	SER	engineered mutation	UNP O66496
D	4237	ALA	GLN	engineered mutation	UNP O66496
E	1011	ASN	CYS	engineered mutation	UNP O66496
E	1235	PRO	SER	engineered mutation	UNP O66496
E	1237	ALA	GLN	engineered mutation	UNP O66496
F	2011	ASN	CYS	engineered mutation	UNP O66496
F	2235	PRO	SER	engineered mutation	UNP O66496
F	2237	ALA	GLN	engineered mutation	UNP O66496
G	3011	ASN	CYS	engineered mutation	UNP O66496
G	3235	PRO	SER	engineered mutation	UNP O66496
G	3237	ALA	GLN	engineered mutation	UNP O66496
H	4011	ASN	CYS	engineered mutation	UNP O66496
H	4235	PRO	SER	engineered mutation	UNP O66496
H	4237	ALA	GLN	engineered mutation	UNP O66496
I	1011	ASN	CYS	engineered mutation	UNP O66496
I	1235	PRO	SER	engineered mutation	UNP O66496
I	1237	ALA	GLN	engineered mutation	UNP O66496
J	2011	ASN	CYS	engineered mutation	UNP O66496
J	2235	PRO	SER	engineered mutation	UNP O66496
J	2237	ALA	GLN	engineered mutation	UNP O66496
K	3011	ASN	CYS	engineered mutation	UNP O66496
K	3235	PRO	SER	engineered mutation	UNP O66496
K	3237	ALA	GLN	engineered mutation	UNP O66496
L	4011	ASN	CYS	engineered mutation	UNP O66496
L	4235	PRO	SER	engineered mutation	UNP O66496
L	4237	ALA	GLN	engineered mutation	UNP O66496

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	I	1	5	4	1	0	0
2	J	1	5	4	1	0	0
2	K	1	5	4	1	0	0
2	L	1	5	4	1	0	0

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	10	3	6	1	0	0
3	B	1	10	3	6	1	0	0
3	C	1	10	3	6	1	0	0
3	D	1	10	3	6	1	0	0
3	E	1	10	3	6	1	0	0
3	F	1	10	3	6	1	0	0
3	G	1	10	3	6	1	0	0
3	H	1	10	3	6	1	0	0
3	I	1	10	3	6	1	0	0
3	J	1	10	3	6	1	0	0
3	K	1	10	3	6	1	0	0
3	L	1	10	3	6	1	0	0

- Molecule 4 is water.

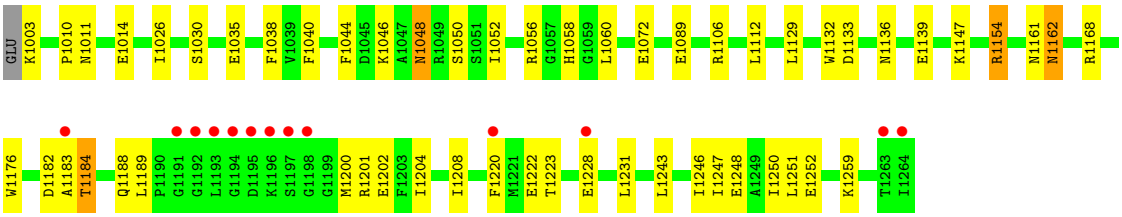
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	185	185	185	0	0
			Total	O		
4	B	190	190	190	0	0
			Total	O		
4	C	107	107	107	0	0
			Total	O		
4	D	75	75	75	0	0
			Total	O		
4	E	64	64	64	0	0
			Total	O		
4	F	54	54	54	0	0
			Total	O		
4	G	178	178	178	0	0
			Total	O		
4	H	170	170	170	0	0
			Total	O		
4	I	185	185	185	0	0
			Total	O		
4	J	172	172	172	0	0
			Total	O		
4	K	50	50	50	0	0
			Total	O		
4	L	99	99	99	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.

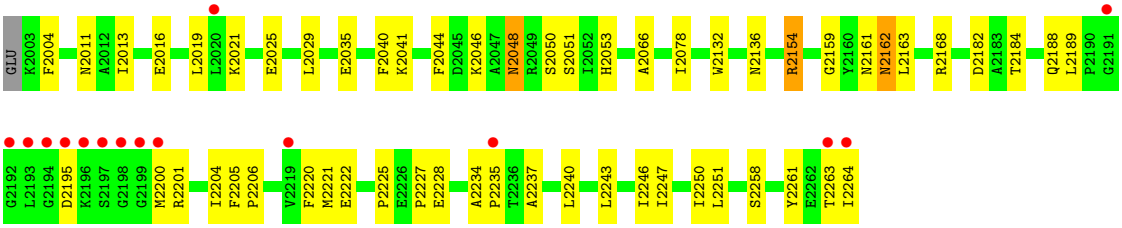
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain A:



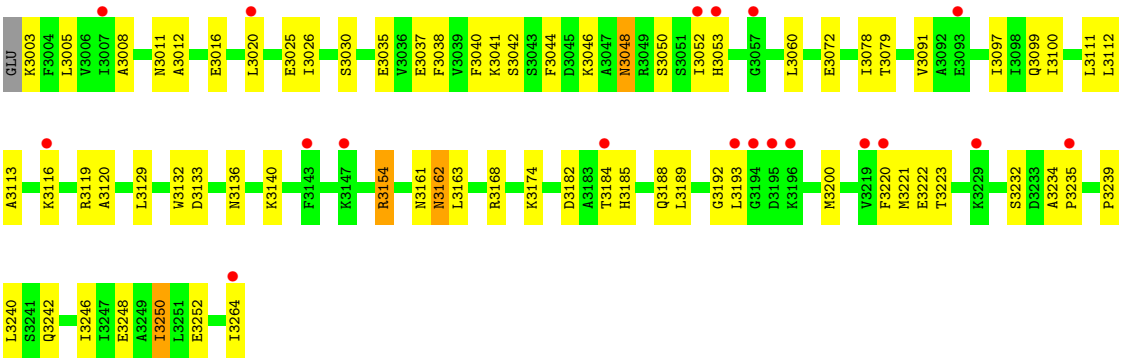
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain B:



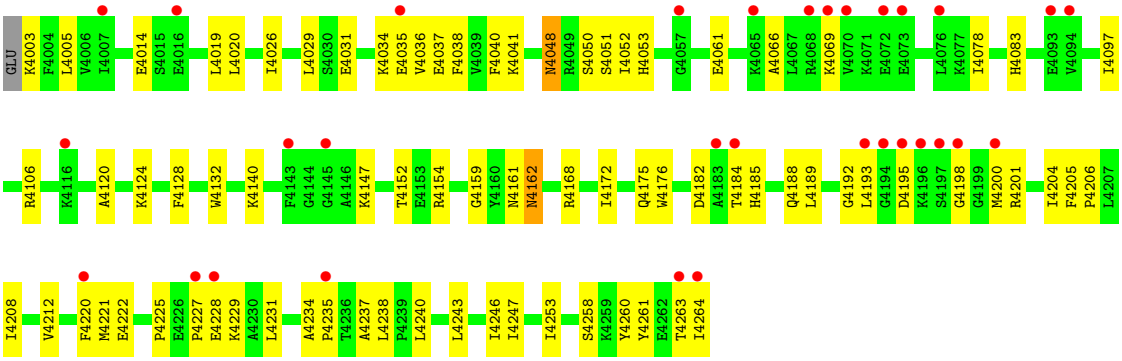
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain C:



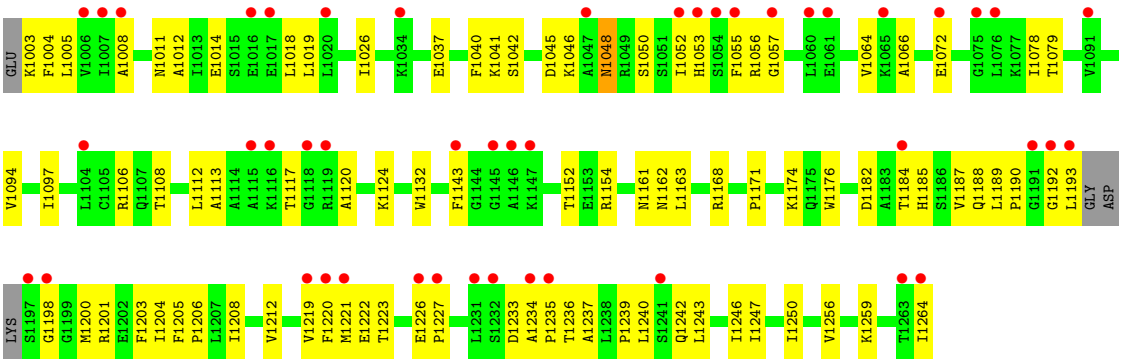
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain D:



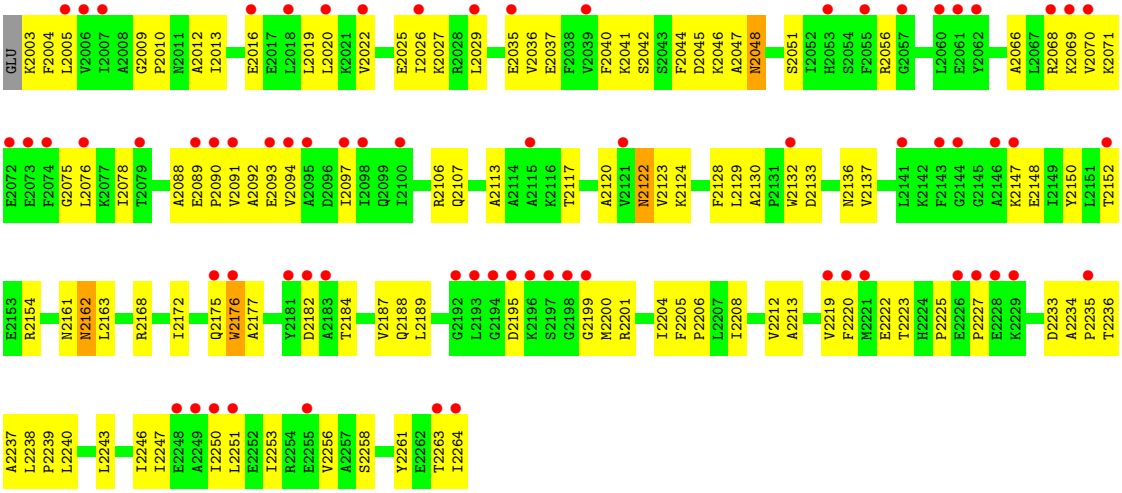
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain E:



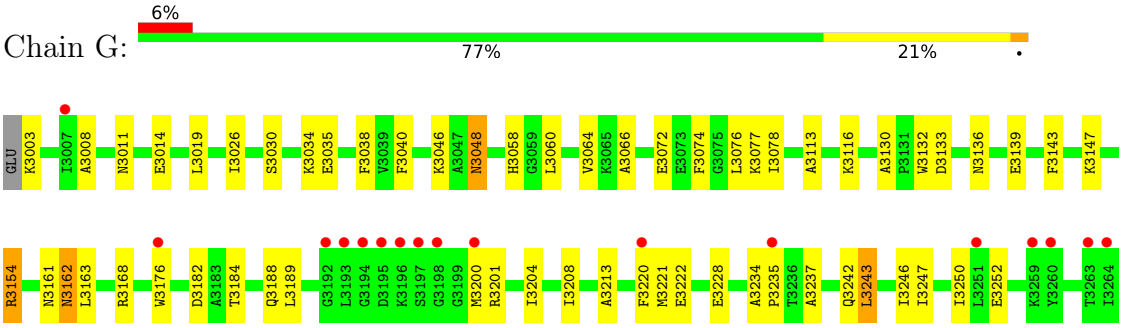
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain F:



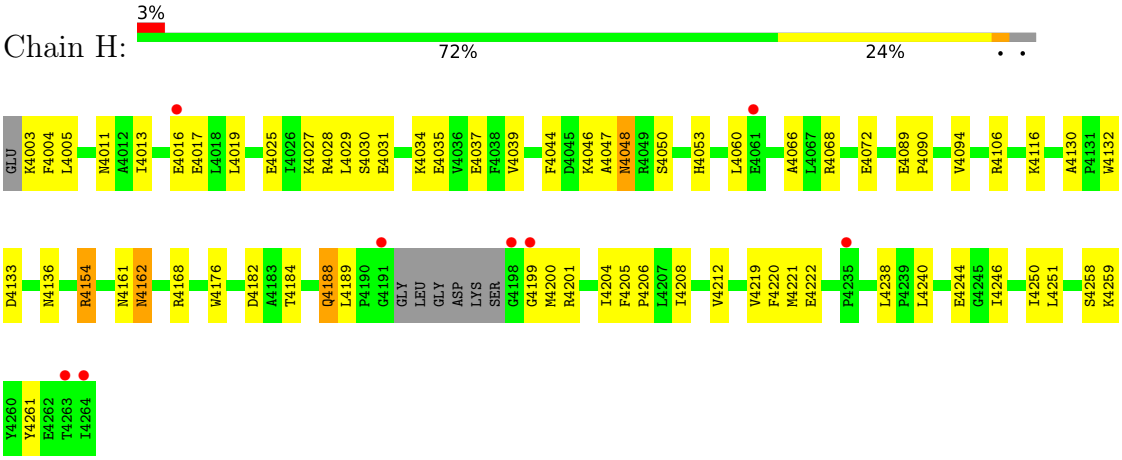
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain G:



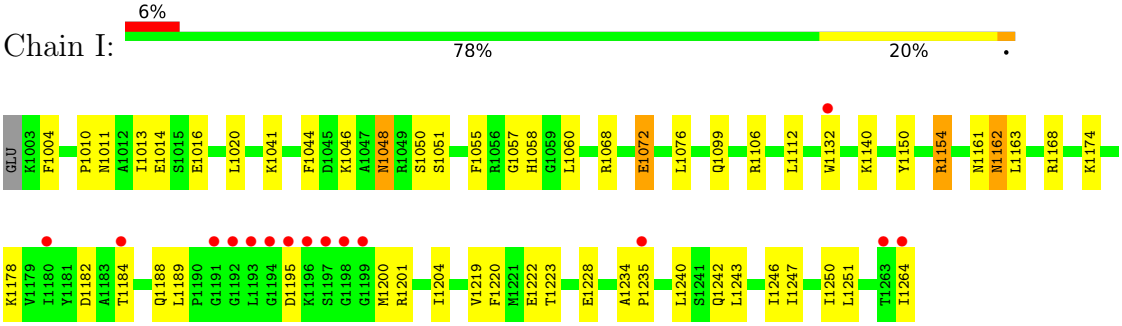
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain H:



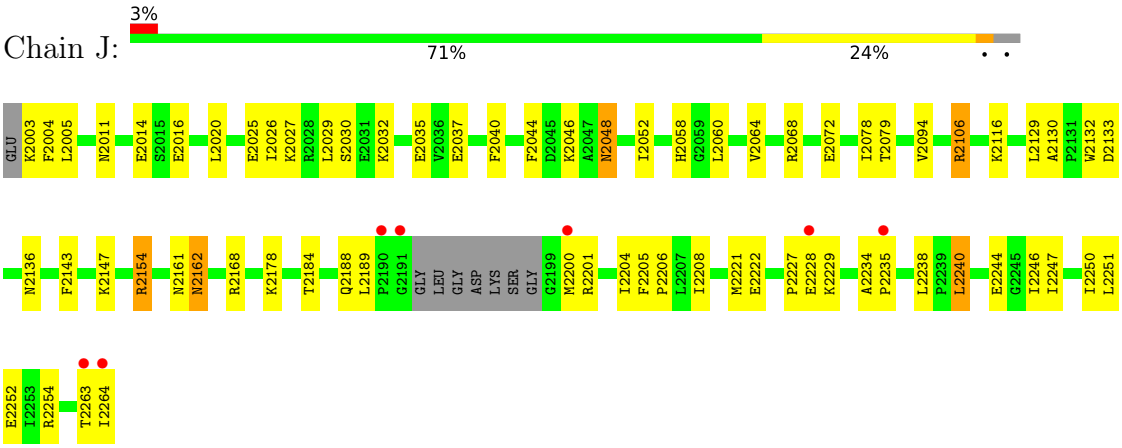
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain I:



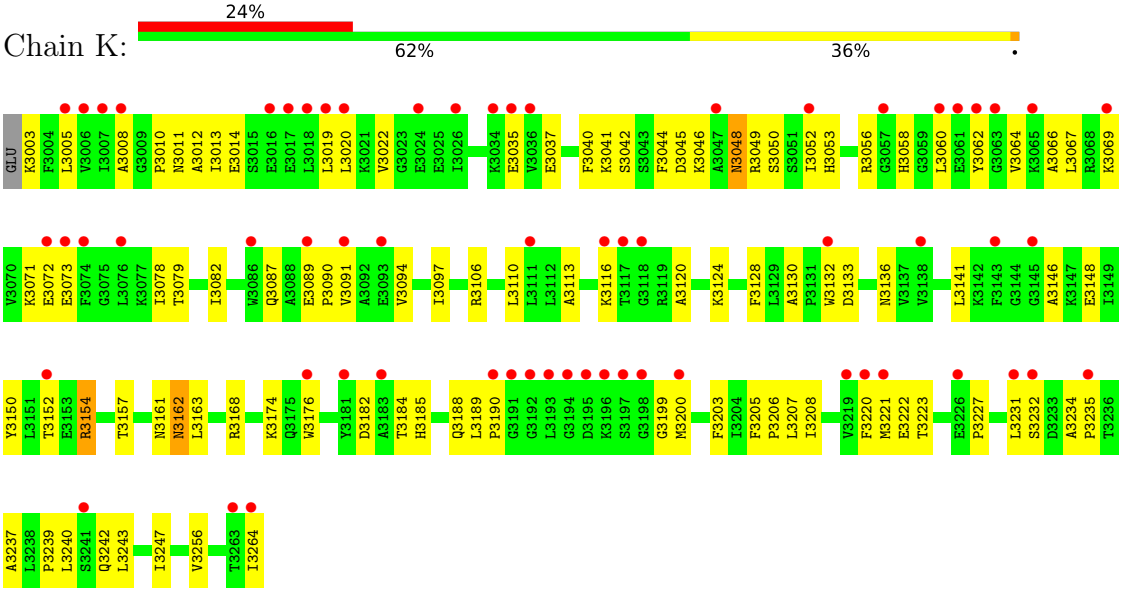
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain J:



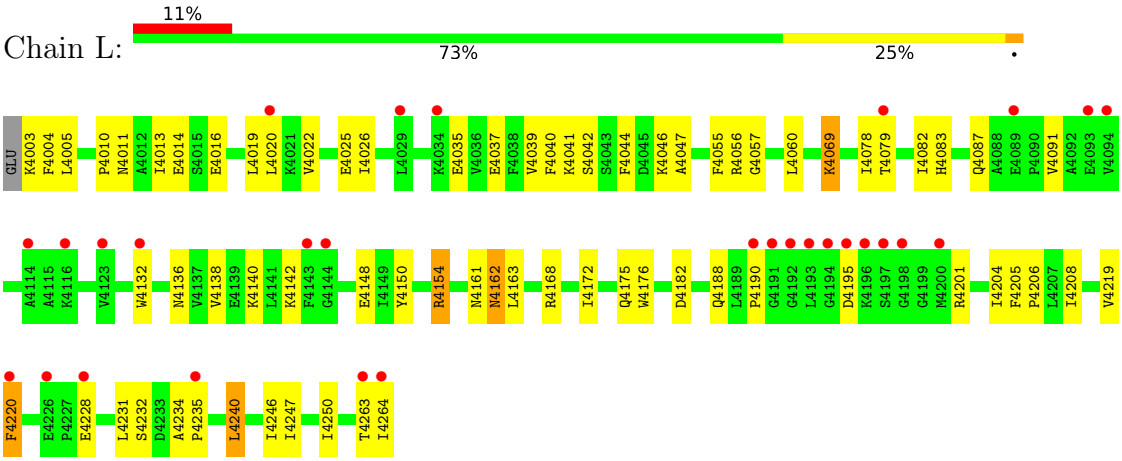
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain K:



• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

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	76.21Å 198.63Å 125.52Å 90.00° 94.28° 90.00°	Depositor
Resolution (Å)	30.18 – 2.11 30.18 – 2.11	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.18-2.11) 91.5 (30.18-2.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.245 0.198 , 0.237	Depositor DCC
R_{free} test set	19281 reflections (9.37%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26278	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4622e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.40	1/2098 (0.0%)	0.60	0/2830
1	B	0.37	0/2098	0.60	0/2830
1	C	0.35	1/2098 (0.0%)	0.53	0/2830
1	D	0.31	0/2098	0.53	0/2830
1	E	0.34	1/2076 (0.0%)	0.52	0/2800
1	F	0.30	0/2098	0.49	0/2830
1	G	0.38	1/2098 (0.0%)	0.59	0/2830
1	H	0.37	0/2058	0.59	0/2776
1	I	0.40	1/2098 (0.0%)	0.60	0/2830
1	J	0.36	0/2054	0.60	0/2771
1	K	0.33	1/2098 (0.0%)	0.50	0/2830
1	L	0.31	0/2098	0.53	0/2830
All	All	0.35	6/25070 (0.0%)	0.56	0/33817

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1072	GLU	CD-OE2	7.41	1.33	1.25
1	G	3072	GLU	CD-OE2	7.40	1.33	1.25
1	E	1072	GLU	CD-OE2	7.16	1.33	1.25
1	K	3072	GLU	CD-OE2	7.08	1.33	1.25
1	I	1072	GLU	CD-OE2	6.91	1.33	1.25
1	C	3072	GLU	CD-OE2	6.81	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2056	0	2095	48	0
1	B	2056	0	2095	54	0
1	C	2056	0	2095	62	0
1	D	2056	0	2095	57	0
1	E	2035	0	2074	64	0
1	F	2056	0	2095	82	0
1	G	2056	0	2095	48	0
1	H	2017	0	2055	63	0
1	I	2056	0	2095	52	0
1	J	2013	0	2052	68	0
1	K	2056	0	2095	70	0
1	L	2056	0	2095	61	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
3	C	10	0	2	0	0
3	D	10	0	2	0	0
3	E	10	0	2	0	0
3	F	10	0	2	0	0
3	G	10	0	2	0	0
3	H	10	0	2	0	0
3	I	10	0	2	0	0
3	J	10	0	2	0	0
3	K	10	0	2	0	0
3	L	10	0	2	0	0
4	A	185	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	190	0	0	2	0
4	C	107	0	0	2	0
4	D	75	0	0	2	0
4	E	64	0	0	5	0
4	F	54	0	0	3	0
4	G	178	0	0	4	0
4	H	170	0	0	7	0
4	I	185	0	0	4	0
4	J	172	0	0	6	0
4	K	50	0	0	3	0
4	L	99	0	0	3	0
All	All	26278	0	25060	676	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 14.

All (676) 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:I:1184:THR:HG21	1:I:1222:GLU:H	1.25	1.01
1:A:1154:ARG:HH22	1:A:1188:GLN:HE22	1.08	1.00
1:B:2184:THR:HG21	1:B:2222:GLU:H	1.20	1.00
1:I:1154:ARG:HH22	1:I:1188:GLN:HE22	1.07	0.99
1:L:4154:ARG:HH22	1:L:4188:GLN:HE22	1.04	0.95
1:C:3154:ARG:HH22	1:C:3188:GLN:HE22	1.14	0.93
1:C:3174:LYS:HG3	1:C:3264:ILE:HD13	1.50	0.92
1:J:2154:ARG:HH22	1:J:2188:GLN:HE22	1.11	0.92
1:H:4184:THR:HG21	1:H:4222:GLU:H	1.38	0.88
1:G:3154:ARG:HH22	1:G:3188:GLN:HE22	1.22	0.87
1:K:3113:ALA:HA	1:K:3116:LYS:HE3	1.55	0.87
1:B:2154:ARG:HH22	1:B:2188:GLN:HE22	1.22	0.85
1:A:1184:THR:HG21	1:A:1222:GLU:H	1.41	0.85
1:H:4154:ARG:HH22	1:H:4188:GLN:HE22	1.25	0.83
1:A:1161:ASN:HD21	1:B:2132:TRP:HE1	1.25	0.83
1:I:1048:ASN:HD22	1:I:1048:ASN:H	1.28	0.82
1:A:1154:ARG:HH22	1:A:1188:GLN:NE2	1.76	0.81
1:H:4205:PHE:O	1:H:4208:ILE:HG22	1.79	0.81
1:L:4205:PHE:O	1:L:4208:ILE:HG22	1.80	0.81
1:I:1184:THR:HG22	4:I:5913:HOH:O	1.78	0.81
1:C:3161:ASN:HD21	1:D:4132:TRP:HE1	1.25	0.80
1:C:3132:TRP:HE1	1:D:4161:ASN:HD21	1.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4185:HIS:O	1:D:4188:GLN:HG2	1.82	0.80
1:H:4244:GLU:HG2	4:H:5021:HOH:O	1.81	0.79
1:L:4154:ARG:HH22	1:L:4188:GLN:NE2	1.79	0.79
1:B:2184:THR:CG2	1:B:2222:GLU:H	1.94	0.79
1:K:3184:THR:HG21	1:K:3222:GLU:H	1.46	0.79
1:J:2025:GLU:HG2	1:J:2240:LEU:HD22	1.63	0.78
1:I:1132:TRP:HE1	1:J:2161:ASN:HD21	1.32	0.77
1:E:1161:ASN:HD21	1:F:2132:TRP:HE1	1.29	0.77
1:A:1132:TRP:HE1	1:B:2161:ASN:HD21	1.30	0.77
1:K:3182:ASP:HA	1:K:3220:PHE:HB3	1.64	0.77
1:I:1161:ASN:HD21	1:J:2132:TRP:HE1	1.34	0.76
1:K:3161:ASN:HD21	1:L:4132:TRP:HE1	1.31	0.76
1:C:3154:ARG:HH22	1:C:3188:GLN:NE2	1.84	0.75
1:G:3132:TRP:HE1	1:H:4161:ASN:HD21	1.32	0.74
1:G:3161:ASN:HD21	1:H:4132:TRP:HE1	1.31	0.74
1:A:1202:GLU:HG3	4:A:5449:HOH:O	1.87	0.73
1:B:2048:ASN:H	1:B:2048:ASN:HD22	1.37	0.73
1:J:2048:ASN:HD22	1:J:2048:ASN:H	1.36	0.72
1:F:2020:LEU:HD21	1:F:2069:LYS:HG3	1.70	0.72
1:D:4184:THR:HG21	1:D:4222:GLU:H	1.53	0.72
1:F:2051:SER:HB2	1:F:2195:ASP:HB2	1.69	0.72
1:K:3174:LYS:HG3	1:K:3264:ILE:HG21	1.70	0.72
1:E:1185:HIS:O	1:E:1188:GLN:HG2	1.90	0.71
1:G:3184:THR:HG21	1:G:3222:GLU:H	1.55	0.71
1:G:3048:ASN:H	1:G:3048:ASN:HD22	1.38	0.71
1:I:1189:LEU:HD21	1:I:1200:MET:HE2	1.73	0.70
1:H:4048:ASN:H	1:H:4048:ASN:HD22	1.39	0.70
1:I:1184:THR:CG2	1:I:1222:GLU:H	2.01	0.70
1:A:1184:THR:HB	4:A:5911:HOH:O	1.91	0.70
1:D:4238:LEU:HD21	1:D:4246:ILE:HD12	1.72	0.70
1:K:3132:TRP:HE1	1:L:4161:ASN:HD21	1.40	0.69
1:J:2154:ARG:HH22	1:J:2188:GLN:NE2	1.88	0.69
1:H:4201:ARG:HG3	1:H:4204:ILE:HD12	1.75	0.69
1:L:4022:VAL:HA	1:L:4240:LEU:HD11	1.75	0.69
1:I:1189:LEU:HD21	1:I:1200:MET:CE	2.23	0.69
1:I:1228:GLU:HG2	4:I:5912:HOH:O	1.91	0.68
1:L:4246:ILE:O	1:L:4250:ILE:HG23	1.93	0.68
1:L:4154:ARG:NH2	1:L:4188:GLN:HE22	1.86	0.68
1:E:1132:TRP:HE1	1:F:2161:ASN:HD21	1.40	0.67
1:B:2051:SER:HB2	1:B:2195:ASP:HB2	1.76	0.67
1:I:1154:ARG:HH22	1:I:1188:GLN:NE2	1.89	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1154:ARG:NH2	1:I:1188:GLN:HE22	1.88	0.66
1:K:3064:VAL:HG13	1:K:3094:VAL:HG11	1.78	0.66
1:A:1136:ASN:HD21	1:B:2195:ASP:HA	1.62	0.65
1:A:1058:HIS:HD2	1:G:3143:PHE:O	1.79	0.65
1:F:2040:PHE:HB3	1:F:2078:ILE:HD13	1.79	0.65
1:E:1097:ILE:HG12	1:E:1120:ALA:HB3	1.77	0.65
1:L:4040:PHE:HB3	1:L:4078:ILE:HD13	1.77	0.65
1:L:4011:ASN:HD22	1:L:4232:SER:HB3	1.61	0.65
1:J:2014:GLU:O	1:J:2058:HIS:HE1	1.80	0.64
1:F:2097:ILE:HG12	1:F:2120:ALA:HB3	1.80	0.64
1:J:2025:GLU:OE2	1:J:2029:LEU:HD21	1.97	0.64
1:E:1048:ASN:H	1:E:1048:ASN:HD22	1.46	0.63
1:C:3189:LEU:HD21	1:C:3200:MET:HE2	1.81	0.63
1:B:2189:LEU:HD21	1:B:2200:MET:CE	2.28	0.63
1:F:2026:ILE:HD12	1:F:2040:PHE:HD1	1.64	0.63
1:C:3182:ASP:HA	1:C:3220:PHE:HB3	1.79	0.63
1:D:4205:PHE:HB3	1:D:4206:PRO:HD3	1.79	0.63
1:L:4154:ARG:HH12	1:L:4188:GLN:HE21	1.47	0.63
1:C:3189:LEU:HD21	1:C:3200:MET:CE	2.28	0.63
1:F:2005:LEU:HD12	1:F:2037:GLU:O	1.99	0.63
1:K:3010:PRO:HD3	1:K:3022:VAL:HG11	1.78	0.63
1:I:1048:ASN:HD22	1:I:1048:ASN:N	1.94	0.62
1:A:1201:ARG:HG3	1:A:1204:ILE:HD12	1.79	0.62
1:G:3014:GLU:O	1:G:3058:HIS:HE1	1.82	0.62
1:K:3234:ALA:N	1:K:3235:PRO:HD2	2.15	0.62
1:D:4227:PRO:HB3	1:D:4237:ALA:HB3	1.82	0.62
1:F:2201:ARG:HG3	1:F:2204:ILE:HD12	1.81	0.62
1:G:3132:TRP:HB3	4:G:6016:HOH:O	1.99	0.62
1:L:4005:LEU:HD12	1:L:4037:GLU:O	1.99	0.62
1:E:1227:PRO:HB3	1:E:1237:ALA:HB3	1.82	0.62
1:J:2068:ARG:O	1:J:2072:GLU:HG3	1.99	0.62
1:L:4025:GLU:HG2	1:L:4240:LEU:HD22	1.82	0.62
1:J:2263:THR:HG22	1:J:2264:ILE:HG22	1.82	0.61
1:A:1014:GLU:HG2	1:A:1231:LEU:HD12	1.82	0.61
1:J:2208:ILE:HD11	1:J:2221:MET:HE3	1.82	0.61
1:B:2154:ARG:HH22	1:B:2188:GLN:NE2	1.96	0.61
1:L:4162:ASN:HD22	1:L:4163:LEU:H	1.46	0.61
1:A:1247:ILE:O	1:A:1250:ILE:HG12	2.00	0.61
1:E:1012:ALA:HB2	1:E:1046:LYS:HD3	1.83	0.61
1:K:3020:LEU:HD21	1:K:3069:LYS:HG3	1.80	0.61
1:E:1162:ASN:HD21	1:H:4168:ARG:HH12	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2027:LYS:HA	1:F:2076:LEU:HD21	1.82	0.61
1:F:2129:LEU:HG	1:F:2133:ASP:HB2	1.83	0.61
1:F:2189:LEU:HD21	1:F:2200:MET:CE	2.31	0.61
1:H:4025:GLU:HG2	1:H:4240:LEU:HD22	1.83	0.61
1:B:2189:LEU:HD21	1:B:2200:MET:HE3	1.82	0.61
1:G:3058:HIS:HD2	1:J:2143:PHE:O	1.83	0.61
1:G:3154:ARG:HH22	1:G:3188:GLN:NE2	1.96	0.61
1:F:2012:ALA:HB2	1:F:2046:LYS:HD3	1.83	0.60
1:D:4189:LEU:HD21	1:D:4200:MET:HE2	1.82	0.60
1:K:3052:ILE:HG23	1:K:3053:HIS:CD2	2.36	0.60
1:A:1048:ASN:H	1:A:1048:ASN:HD22	1.48	0.60
1:I:1201:ARG:HG3	1:I:1204:ILE:HD12	1.84	0.60
1:E:1182:ASP:HA	1:E:1220:PHE:HB3	1.84	0.60
1:C:3162:ASN:HD22	1:C:3163:LEU:H	1.48	0.60
1:D:4263:THR:HG22	1:D:4264:ILE:HG22	1.82	0.60
1:F:2004:PHE:HE1	1:F:2250:ILE:HD12	1.67	0.60
1:B:2201:ARG:HG3	1:B:2204:ILE:HD12	1.84	0.60
1:G:3136:ASN:HB3	1:H:4050:SER:O	2.02	0.60
1:K:3205:PHE:O	1:K:3208:ILE:HG22	2.01	0.60
1:K:3005:LEU:HD12	1:K:3037:GLU:O	2.02	0.59
1:K:3019:LEU:HD22	1:K:3066:ALA:HB1	1.85	0.59
1:L:4041:LYS:HD3	1:L:4042:SER:N	2.17	0.59
1:C:3011:ASN:HD21	1:C:3046:LYS:HE2	1.66	0.59
1:C:3113:ALA:O	1:C:3116:LYS:HG2	2.03	0.59
1:C:3239:PRO:HG2	1:C:3242:GLN:NE2	2.17	0.59
1:C:3012:ALA:HB2	1:C:3046:LYS:HD3	1.83	0.59
1:E:1184:THR:HG21	1:E:1222:GLU:H	1.67	0.59
1:F:2238:LEU:HD12	1:F:2239:PRO:HD2	1.84	0.59
1:K:3184:THR:CG2	1:K:3222:GLU:H	2.15	0.59
1:D:4014:GLU:HG2	1:D:4231:LEU:HD12	1.85	0.59
1:A:1189:LEU:HD21	1:A:1200:MET:CE	2.33	0.59
1:L:4247:ILE:O	1:L:4250:ILE:HG12	2.03	0.59
1:C:3099:GLN:HE22	1:C:3220:PHE:HE2	1.49	0.58
1:C:3011:ASN:ND2	1:C:3232:SER:OG	2.36	0.58
1:J:2154:ARG:HH12	1:J:2188:GLN:HE21	1.51	0.58
1:J:2247:ILE:O	1:J:2250:ILE:HG12	2.02	0.58
1:H:4184:THR:CG2	1:H:4222:GLU:H	2.14	0.58
1:H:4130:ALA:HB3	1:H:4133:ASP:OD2	2.04	0.58
1:H:4259:LYS:HB2	4:H:5614:HOH:O	2.03	0.58
1:E:1045:ASP:HA	1:E:1056:ARG:O	2.04	0.58
1:H:4005:LEU:HD12	1:H:4037:GLU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3052:ILE:HB	1:L:4140:LYS:HG2	1.85	0.58
1:K:3064:VAL:HG13	1:K:3094:VAL:CG1	2.34	0.57
1:K:3227:PRO:HB3	1:K:3237:ALA:HB3	1.85	0.57
1:D:4040:PHE:HB3	1:D:4078:ILE:HD13	1.85	0.57
1:H:4184:THR:HG21	1:H:4222:GLU:N	2.15	0.57
1:B:2168:ARG:HH12	1:C:3162:ASN:HD21	1.52	0.57
1:F:2124:LYS:HD3	1:F:2152:THR:HB	1.87	0.57
1:G:3162:ASN:HD22	1:G:3163:LEU:H	1.53	0.57
1:B:2184:THR:HG21	1:B:2222:GLU:N	2.04	0.57
1:D:4147:LYS:NZ	1:D:4147:LYS:HB3	2.19	0.57
1:F:2223:THR:OG1	1:F:2243:LEU:HD11	2.05	0.57
1:I:1182:ASP:HA	1:I:1220:PHE:HB3	1.87	0.57
1:H:4068:ARG:HE	1:H:4094:VAL:HG22	1.68	0.57
1:C:3011:ASN:HD21	1:C:3046:LYS:CE	2.17	0.57
1:I:1154:ARG:HH12	1:I:1188:GLN:NE2	2.02	0.57
1:E:1106:ARG:HB2	4:E:5426:HOH:O	2.05	0.56
1:L:4205:PHE:HB3	1:L:4206:PRO:HD3	1.86	0.56
1:J:2205:PHE:HB3	1:J:2206:PRO:HD3	1.87	0.56
1:B:2247:ILE:O	1:B:2250:ILE:HG12	2.05	0.56
1:F:2189:LEU:HD21	1:F:2200:MET:HE2	1.88	0.56
1:L:4069:LYS:HB2	1:L:4069:LYS:NZ	2.20	0.56
1:C:3005:LEU:HD12	1:C:3037:GLU:O	2.05	0.56
1:J:2189:LEU:HD21	1:J:2200:MET:CE	2.35	0.56
1:K:3044:PHE:CZ	1:K:3060:LEU:HD13	2.41	0.56
1:E:1239:PRO:HG2	1:E:1242:GLN:NE2	2.20	0.56
1:I:1184:THR:HG21	1:I:1222:GLU:N	2.09	0.56
1:F:2026:ILE:HD12	1:F:2040:PHE:CD1	2.40	0.56
1:J:2208:ILE:CD1	1:J:2221:MET:HE3	2.35	0.56
1:K:3045:ASP:HA	1:K:3056:ARG:O	2.06	0.56
1:K:3050:SER:O	1:L:4136:ASN:HB3	2.06	0.56
1:G:3189:LEU:HD21	1:G:3200:MET:CE	2.36	0.55
1:D:4019:LEU:HD12	1:D:4066:ALA:HB1	1.88	0.55
1:H:4259:LYS:HE2	4:H:5395:HOH:O	2.06	0.55
1:F:2233:ASP:HB3	1:F:2236:THR:OG1	2.06	0.55
1:A:1184:THR:CG2	1:A:1222:GLU:H	2.17	0.55
1:G:3154:ARG:HH12	1:G:3188:GLN:HE21	1.54	0.55
1:I:1223:THR:OG1	1:I:1243:LEU:HD11	2.06	0.55
1:H:4031:GLU:O	1:H:4034:LYS:HE2	2.06	0.55
1:D:4201:ARG:HG3	1:D:4204:ILE:HD12	1.89	0.55
1:E:1052:ILE:HG23	1:E:1053:HIS:CD2	2.42	0.55
1:D:4005:LEU:HD12	1:D:4037:GLU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1011:ASN:HD21	1:E:1046:LYS:HE2	1.72	0.55
1:E:1048:ASN:HD22	1:E:1048:ASN:N	2.04	0.55
1:D:4061:GLU:HB3	4:D:6178:HOH:O	2.05	0.55
1:L:4182:ASP:HA	1:L:4220:PHE:HB3	1.89	0.55
1:D:4204:ILE:O	1:D:4208:ILE:HG13	2.07	0.55
1:F:2147:LYS:NZ	1:F:2147:LYS:HB3	2.22	0.55
1:G:3182:ASP:HA	1:G:3220:PHE:HB3	1.89	0.55
1:A:1003:LYS:HD2	1:A:1035:GLU:O	2.07	0.54
1:H:4027:LYS:O	1:H:4030:SER:HB3	2.06	0.54
1:A:1154:ARG:HH12	1:A:1188:GLN:HE21	1.56	0.54
1:H:4189:LEU:HD21	1:H:4200:MET:CE	2.37	0.54
1:F:2234:ALA:N	1:F:2235:PRO:HD2	2.22	0.54
1:G:3247:ILE:O	1:G:3250:ILE:HG12	2.06	0.54
1:L:4263:THR:HG22	1:L:4264:ILE:HG22	1.89	0.54
1:C:3248:GLU:O	1:C:3252:GLU:HG3	2.08	0.54
1:G:3011:ASN:HD21	1:G:3046:LYS:NZ	2.06	0.54
1:J:2025:GLU:O	1:J:2029:LEU:HD23	2.08	0.54
1:L:4014:GLU:OE2	1:L:4231:LEU:HG	2.07	0.54
1:C:3162:ASN:ND2	1:C:3163:LEU:H	2.06	0.54
1:F:2148:GLU:HG2	1:F:2150:TYR:HE1	1.73	0.54
1:F:2243:LEU:O	1:F:2247:ILE:HG13	2.08	0.54
1:I:1011:ASN:HD21	1:I:1046:LYS:CE	2.19	0.54
1:K:3189:LEU:HD21	1:K:3200:MET:HE2	1.90	0.54
1:F:2130:ALA:HB3	1:F:2133:ASP:OD2	2.08	0.53
1:L:4004:PHE:HZ	1:L:4219:VAL:HG23	1.73	0.53
1:F:2204:ILE:O	1:F:2208:ILE:HG13	2.07	0.53
1:H:4182:ASP:HA	1:H:4220:PHE:HB3	1.90	0.53
1:J:2026:ILE:HD12	1:J:2040:PHE:CD1	2.43	0.53
1:A:1011:ASN:HD21	1:A:1046:LYS:NZ	2.06	0.53
1:B:2205:PHE:HB3	1:B:2206:PRO:HD3	1.88	0.53
1:C:3041:LYS:HD3	1:C:3041:LYS:C	2.29	0.53
1:F:2025:GLU:OE2	1:F:2029:LEU:HD13	2.07	0.53
1:J:2027:LYS:O	1:J:2030:SER:HB3	2.08	0.53
1:A:1250:ILE:HG13	1:A:1251:LEU:N	2.24	0.53
1:C:3184:THR:HG21	1:C:3222:GLU:H	1.74	0.53
1:L:4041:LYS:HD3	1:L:4041:LYS:C	2.29	0.53
1:D:4189:LEU:HD21	1:D:4200:MET:CE	2.39	0.53
1:J:2201:ARG:HG3	1:J:2204:ILE:HD12	1.89	0.53
1:L:4201:ARG:HG3	1:L:4204:ILE:HD12	1.89	0.53
1:E:1008:ALA:HA	1:E:1221:MET:O	2.09	0.53
1:G:3034:LYS:HE3	4:G:6657:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2162:ASN:HD21	1:K:3168:ARG:HH12	1.56	0.53
1:D:4003:LYS:HB2	1:D:4035:GLU:O	2.10	0.52
1:D:4243:LEU:O	1:D:4247:ILE:HG13	2.09	0.52
1:H:4116:LYS:HD3	4:H:6093:HOH:O	2.09	0.52
1:K:3174:LYS:HG3	1:K:3264:ILE:HD13	1.91	0.52
1:H:4025:GLU:O	1:H:4029:LEU:HD22	2.09	0.52
1:A:1248:GLU:O	1:A:1252:GLU:HG3	2.09	0.52
1:E:1162:ASN:ND2	1:E:1163:LEU:H	2.07	0.52
1:I:1240:LEU:O	1:I:1243:LEU:HD13	2.09	0.52
1:F:2091:VAL:C	1:F:2093:GLU:H	2.12	0.52
1:C:3041:LYS:HD3	1:C:3042:SER:N	2.24	0.52
1:J:2246:ILE:O	1:J:2250:ILE:HG23	2.10	0.52
1:K:3189:LEU:HD21	1:K:3200:MET:CE	2.39	0.52
1:G:3237:ALA:HB2	4:G:5922:HOH:O	2.08	0.52
1:I:1106:ARG:HA	4:I:5303:HOH:O	2.09	0.52
1:J:2234:ALA:N	1:J:2235:PRO:HD2	2.25	0.52
1:C:3040:PHE:HB3	1:C:3078:ILE:HD13	1.91	0.52
1:C:3140:LYS:HG2	1:D:4052:ILE:HB	1.91	0.52
1:K:3162:ASN:HD22	1:K:3163:LEU:H	1.58	0.52
1:A:1014:GLU:O	1:A:1058:HIS:HE1	1.93	0.52
1:H:4068:ARG:HH21	1:H:4094:VAL:HG23	1.75	0.52
1:D:4234:ALA:N	1:D:4235:PRO:HD2	2.25	0.51
1:I:1154:ARG:HH12	1:I:1188:GLN:HE21	1.56	0.51
1:K:3003:LYS:HG3	1:K:3035:GLU:O	2.10	0.51
1:K:3243:LEU:O	1:K:3247:ILE:HG13	2.10	0.51
1:H:4028:ARG:HH22	1:H:4244:GLU:CD	2.13	0.51
1:I:1168:ARG:HH12	1:L:4162:ASN:HD21	1.59	0.51
1:A:1189:LEU:HD21	1:A:1200:MET:HE2	1.93	0.51
1:C:3264:ILE:HG13	1:C:3264:ILE:OXT	2.11	0.51
1:D:4264:ILE:HG23	1:D:4264:ILE:OXT	2.11	0.51
1:D:4031:GLU:HA	1:D:4034:LYS:HE2	1.92	0.51
1:J:2032:LYS:HE2	1:J:2244:GLU:OE2	2.11	0.51
1:A:1129:LEU:HG	1:A:1133:ASP:HB2	1.93	0.50
1:B:2240:LEU:O	1:B:2243:LEU:HD13	2.11	0.50
1:E:1064:VAL:HG13	1:E:1094:VAL:CG1	2.41	0.50
1:B:2040:PHE:HB3	1:B:2078:ILE:HD13	1.93	0.50
1:J:2011:ASN:HD21	1:J:2046:LYS:CE	2.24	0.50
1:F:2045:ASP:HA	1:F:2056:ARG:O	2.12	0.50
1:G:3048:ASN:HD22	1:G:3048:ASN:N	2.02	0.50
1:J:2116:LYS:HE2	4:J:6485:HOH:O	2.12	0.50
1:A:1044:PHE:CZ	1:A:1060:LEU:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1234:ALA:N	1:E:1235:PRO:HD2	2.26	0.50
1:F:2113:ALA:O	1:F:2117:THR:HG23	2.11	0.50
1:L:4016:GLU:O	1:L:4020:LEU:HG	2.12	0.50
1:H:4068:ARG:O	1:H:4072:GLU:HG3	2.12	0.50
1:H:4189:LEU:HD21	1:H:4200:MET:HE1	1.94	0.50
1:K:3014:GLU:HG2	1:K:3231:LEU:HD12	1.94	0.50
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.09	0.50
1:E:1193:LEU:HD13	1:E:1198:GLY:HA3	1.93	0.50
1:K:3041:LYS:HD3	1:K:3042:SER:N	2.27	0.50
1:B:2184:THR:HG23	1:B:2221:MET:HA	1.92	0.50
1:E:1223:THR:OG1	1:E:1240:LEU:HA	2.12	0.50
1:A:1154:ARG:O	1:A:1154:ARG:HD3	2.12	0.50
1:B:2154:ARG:HH12	1:B:2188:GLN:HE21	1.60	0.50
1:G:3130:ALA:HB3	1:G:3133:ASP:OD2	2.12	0.50
1:C:3234:ALA:N	1:C:3235:PRO:HD2	2.27	0.49
1:E:1048:ASN:HB3	1:F:2107:GLN:HE22	1.76	0.49
1:J:2228:GLU:HG2	1:J:2229:LYS:N	2.27	0.49
1:B:2011:ASN:HD21	1:B:2046:LYS:CE	2.26	0.49
1:I:1004:PHE:CE1	1:I:1250:ILE:HD12	2.47	0.49
1:L:4162:ASN:HD22	1:L:4163:LEU:N	2.10	0.49
1:C:3060:LEU:HD11	1:C:3091:VAL:HG22	1.93	0.49
1:E:1233:ASP:HB3	1:E:1236:THR:OG1	2.12	0.49
1:F:2128:PHE:HB3	4:F:5298:HOH:O	2.10	0.49
1:I:1140:LYS:HG2	1:J:2052:ILE:HB	1.94	0.49
1:F:2106:ARG:HB2	4:F:5300:HOH:O	2.13	0.49
1:J:2154:ARG:HH12	1:J:2188:GLN:NE2	2.10	0.49
1:B:2246:ILE:O	1:B:2250:ILE:HG23	2.13	0.49
1:I:1013:ILE:HD12	1:I:1044:PHE:HA	1.94	0.49
1:I:1099:GLN:HE22	1:I:1220:PHE:HE2	1.60	0.49
1:A:1136:ASN:HB3	1:B:2050:SER:O	2.12	0.49
1:C:3011:ASN:HB3	4:C:5578:HOH:O	2.12	0.49
1:J:2005:LEU:HD12	1:J:2037:GLU:O	2.12	0.49
1:J:2052:ILE:HG13	1:J:2052:ILE:O	2.11	0.49
1:E:1078:ILE:HG22	1:E:1079:THR:N	2.28	0.49
1:H:4208:ILE:HD11	1:H:4219:VAL:HG11	1.95	0.49
1:H:4005:LEU:HD11	1:H:4039:VAL:HG23	1.95	0.49
1:J:2221:MET:HE2	1:J:2238:LEU:CD2	2.42	0.49
1:H:4212:VAL:HG11	1:H:4250:ILE:HB	1.95	0.49
1:I:1011:ASN:HD21	1:I:1046:LYS:NZ	2.11	0.49
1:I:1068:ARG:O	1:I:1072:GLU:HG3	2.13	0.49
1:C:3136:ASN:HB3	1:D:4050:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1108:THR:O	1:E:1112:LEU:HD13	2.12	0.49
1:E:1247:ILE:O	1:E:1250:ILE:HG12	2.12	0.49
1:F:2088:ALA:HB2	1:F:2113:ALA:HB1	1.95	0.49
1:G:3003:LYS:HG3	1:G:3035:GLU:O	2.13	0.49
1:K:3040:PHE:HB3	1:K:3078:ILE:HD13	1.93	0.49
1:A:1162:ASN:HD21	1:D:4168:ARG:HH12	1.61	0.48
1:B:2189:LEU:HD11	1:B:2200:MET:CE	2.43	0.48
1:C:3030:SER:HA	1:C:3038:PHE:CE1	2.48	0.48
1:H:4048:ASN:HD22	1:H:4048:ASN:N	2.02	0.48
1:L:4026:ILE:HD12	1:L:4040:PHE:CD1	2.48	0.48
1:E:1187:VAL:HG21	1:E:1204:ILE:HG12	1.95	0.48
1:K:3041:LYS:HD3	1:K:3041:LYS:C	2.33	0.48
1:B:2263:THR:HG22	1:B:2264:ILE:N	2.29	0.48
1:H:4016:GLU:HG3	1:H:4017:GLU:N	2.27	0.48
1:A:1026:ILE:HD12	1:A:1040:PHE:CD1	2.48	0.48
1:A:1050:SER:O	1:B:2136:ASN:HB3	2.13	0.48
1:L:4087:GLN:O	1:L:4091:VAL:HG23	2.12	0.48
1:F:2066:ALA:O	1:F:2070:VAL:HG23	2.13	0.48
1:F:2162:ASN:HD22	1:F:2163:LEU:H	1.62	0.48
1:K:3011:ASN:ND2	1:K:3232:SER:OG	2.44	0.48
1:K:3190:PRO:HG3	4:K:5774:HOH:O	2.14	0.48
1:A:1052:ILE:HG13	1:A:1052:ILE:O	2.14	0.48
1:B:2240:LEU:HA	1:B:2243:LEU:HD13	1.96	0.48
1:E:1041:LYS:HD3	1:E:1042:SER:N	2.29	0.48
1:E:1064:VAL:HG13	1:E:1094:VAL:HG11	1.96	0.48
1:H:4003:LYS:HB2	1:H:4035:GLU:O	2.13	0.48
1:I:1004:PHE:HZ	1:I:1219:VAL:HG13	1.79	0.48
1:B:2025:GLU:HG2	1:B:2240:LEU:HD22	1.95	0.48
1:E:1204:ILE:O	1:E:1208:ILE:HG13	2.13	0.48
1:F:2238:LEU:HD21	1:F:2246:ILE:HD12	1.95	0.48
1:F:2246:ILE:O	1:F:2250:ILE:HG23	2.13	0.48
1:G:3234:ALA:N	1:G:3235:PRO:HD2	2.29	0.48
1:H:4205:PHE:HB3	1:H:4206:PRO:HD3	1.96	0.48
1:K:3071:LYS:HB2	1:K:3078:ILE:CG1	2.44	0.48
1:B:2237:ALA:HB3	4:B:5271:HOH:O	2.13	0.47
1:C:3044:PHE:CZ	1:C:3060:LEU:HD13	2.49	0.47
1:E:1171:PRO:HB3	4:E:5791:HOH:O	2.13	0.47
1:H:4116:LYS:O	1:H:4116:LYS:HG2	2.13	0.47
1:A:1147:LYS:HE2	4:A:6631:HOH:O	2.13	0.47
1:F:2027:LYS:HB3	4:F:6324:HOH:O	2.15	0.47
1:F:2176:TRP:O	1:F:2177:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2184:THR:HG21	1:F:2222:GLU:H	1.78	0.47
1:K:3128:PHE:HB3	4:L:5468:HOH:O	2.15	0.47
1:L:4003:LYS:HB2	1:L:4035:GLU:O	2.14	0.47
1:A:1168:ARG:HH12	1:D:4162:ASN:HD21	1.61	0.47
1:E:1003:LYS:N	4:E:5833:HOH:O	2.47	0.47
1:J:2201:ARG:HH22	1:J:2227:PRO:HB2	1.78	0.47
1:E:1124:LYS:HD3	1:E:1152:THR:HB	1.96	0.47
1:J:2011:ASN:HD21	1:J:2046:LYS:HE2	1.80	0.47
1:L:4044:PHE:CZ	1:L:4060:LEU:HD13	2.50	0.47
1:D:4212:VAL:HG23	1:D:4253:ILE:HG21	1.97	0.47
1:E:1026:ILE:HD12	1:E:1040:PHE:HD1	1.79	0.47
1:E:1174:LYS:HG3	1:E:1264:ILE:HD13	1.96	0.47
1:I:1247:ILE:O	1:I:1250:ILE:HG12	2.14	0.47
1:C:3078:ILE:HG22	1:C:3079:THR:N	2.29	0.47
1:E:1014:GLU:OE1	1:E:1018:LEU:HD22	2.15	0.47
1:E:1242:GLN:O	1:E:1246:ILE:HG12	2.14	0.47
1:F:2188:GLN:HA	1:F:2199:GLY:HA2	1.96	0.47
1:G:3030:SER:HA	1:G:3038:PHE:CE1	2.50	0.47
1:G:3204:ILE:O	1:G:3208:ILE:HG13	2.15	0.47
1:C:3100:ILE:HG13	1:C:3111:LEU:HD23	1.96	0.47
1:D:4036:VAL:HB	1:D:4038:PHE:CE1	2.49	0.47
1:F:2123:VAL:HG11	1:F:2137:VAL:HG11	1.97	0.47
1:H:4013:ILE:HD12	1:H:4044:PHE:HA	1.96	0.47
1:H:4068:ARG:HE	1:H:4094:VAL:CG2	2.28	0.47
1:J:2154:ARG:NH2	1:J:2188:GLN:HE22	1.94	0.47
1:K:3012:ALA:HB2	1:K:3046:LYS:HD3	1.96	0.47
1:K:3130:ALA:HB3	1:K:3133:ASP:OD2	2.14	0.47
1:D:4172:ILE:O	1:D:4175:GLN:HG3	2.15	0.47
1:D:4228:GLU:HG3	1:D:4229:LYS:HG3	1.97	0.47
1:H:4201:ARG:HA	1:H:4204:ILE:HG13	1.96	0.47
1:K:3154:ARG:O	1:K:3154:ARG:HD3	2.14	0.47
1:C:3246:ILE:O	1:C:3250:ILE:HG12	2.14	0.47
1:E:1205:PHE:N	1:E:1206:PRO:HD2	2.30	0.47
1:E:1246:ILE:O	1:E:1250:ILE:HG23	2.15	0.47
1:J:2004:PHE:HB2	1:J:2254:ARG:NH1	2.29	0.47
1:J:2129:LEU:HG	1:J:2133:ASP:HB2	1.96	0.47
1:J:2184:THR:HG21	1:J:2222:GLU:H	1.80	0.47
1:K:3239:PRO:HG2	1:K:3242:GLN:NE2	2.30	0.47
1:F:2182:ASP:HA	1:F:2220:PHE:HB3	1.97	0.47
1:I:1004:PHE:CZ	1:I:1219:VAL:HG13	2.50	0.47
1:J:2048:ASN:HD22	1:J:2048:ASN:N	2.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2178:LYS:HD3	4:J:5643:HOH:O	2.14	0.47
1:J:2201:ARG:NH2	1:J:2227:PRO:HB2	2.29	0.47
1:L:4172:ILE:O	1:L:4175:GLN:HG3	2.15	0.47
1:C:3182:ASP:OD2	1:C:3185:HIS:ND1	2.48	0.46
1:F:2041:LYS:C	1:F:2041:LYS:HD3	2.35	0.46
1:K:3234:ALA:N	1:K:3235:PRO:CD	2.78	0.46
1:A:1056:ARG:HH11	1:G:3147:LYS:NZ	2.13	0.46
4:C:5408:HOH:O	1:D:4083:HIS:HD2	1.99	0.46
1:I:1011:ASN:HD21	1:I:1046:LYS:HE2	1.80	0.46
1:K:3078:ILE:HG22	1:K:3079:THR:N	2.30	0.46
1:K:3203:PHE:O	1:K:3207:LEU:HG	2.15	0.46
1:A:1132:TRP:HE1	1:B:2161:ASN:ND2	2.07	0.46
1:K:3058:HIS:HB2	1:K:3062:TYR:CD2	2.50	0.46
1:L:4016:GLU:HG2	1:L:4020:LEU:HD11	1.97	0.46
1:E:1256:VAL:O	1:E:1259:LYS:HG2	2.15	0.46
1:H:4003:LYS:N	4:H:5282:HOH:O	2.48	0.46
1:A:1136:ASN:ND2	1:B:2195:ASP:HA	2.30	0.46
1:E:1243:LEU:O	1:E:1247:ILE:HG13	2.15	0.46
1:F:2041:LYS:HD3	1:F:2042:SER:N	2.30	0.46
1:F:2089:GLU:N	1:F:2090:PRO:HD2	2.29	0.46
1:G:3048:ASN:H	1:G:3048:ASN:ND2	2.10	0.46
1:I:1014:GLU:O	1:I:1058:HIS:HE1	1.99	0.46
1:D:4184:THR:CG2	1:D:4222:GLU:H	2.23	0.46
1:D:4193:LEU:HD23	1:D:4198:GLY:HA3	1.97	0.46
1:E:1143:PHE:HA	4:E:6307:HOH:O	2.15	0.46
1:J:2201:ARG:HA	1:J:2204:ILE:HG13	1.97	0.46
1:K:3136:ASN:HD21	1:L:4195:ASP:HA	1.81	0.46
1:L:4162:ASN:ND2	1:L:4163:LEU:H	2.13	0.46
1:L:4201:ARG:HA	1:L:4204:ILE:HG13	1.98	0.46
1:H:4011:ASN:HD21	1:H:4046:LYS:HE2	1.81	0.46
1:K:3067:LEU:HB3	1:K:3078:ILE:HG21	1.98	0.46
1:H:4089:GLU:HB3	1:H:4090:PRO:CD	2.46	0.46
1:E:1193:LEU:HD13	1:E:1198:GLY:CA	2.45	0.46
1:J:2003:LYS:CA	4:J:5093:HOH:O	2.64	0.46
1:A:1056:ARG:NH1	1:G:3147:LYS:HE2	2.31	0.45
1:D:4048:ASN:H	1:D:4048:ASN:HD22	1.64	0.45
1:D:4221:MET:CE	1:D:4238:LEU:HD22	2.45	0.45
1:F:2010:PRO:HD3	1:F:2022:VAL:HG11	1.98	0.45
1:F:2238:LEU:HD21	1:F:2246:ILE:CD1	2.46	0.45
1:H:4068:ARG:HH21	1:H:4094:VAL:CG2	2.29	0.45
1:B:2019:LEU:HD12	1:B:2066:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3052:ILE:HB	1:D:4140:LYS:HG2	1.98	0.45
1:A:1011:ASN:HD21	1:A:1046:LYS:CE	2.29	0.45
1:B:2162:ASN:HD21	1:C:3168:ARG:HH12	1.63	0.45
1:C:3050:SER:OG	1:D:4106:ARG:NH1	2.48	0.45
1:D:4052:ILE:HG23	1:D:4053:HIS:CD2	2.51	0.45
1:I:1162:ASN:HD21	1:L:4168:ARG:HH12	1.62	0.45
1:A:1246:ILE:O	1:A:1250:ILE:HG23	2.17	0.45
1:C:3154:ARG:HH12	1:C:3188:GLN:HE21	1.64	0.45
1:F:2205:PHE:HB3	1:F:2206:PRO:HD3	1.99	0.45
1:F:2212:VAL:HG23	1:F:2253:ILE:HG21	1.98	0.45
1:H:4154:ARG:HH22	1:H:4188:GLN:NE2	2.04	0.45
1:H:4004:PHE:CE1	1:H:4250:ILE:HD12	2.51	0.45
1:L:4082:ILE:HG22	1:L:4091:VAL:HG21	1.98	0.45
1:E:1192:GLY:C	1:E:1193:LEU:HD12	2.36	0.45
1:F:2019:LEU:HB3	1:F:2070:VAL:HG21	1.98	0.45
1:F:2258:SER:HA	1:F:2261:TYR:CE2	2.52	0.45
1:J:2250:ILE:HG13	1:J:2251:LEU:N	2.30	0.45
1:L:4010:PRO:HG3	1:L:4019:LEU:HD23	1.97	0.45
1:F:2225:PRO:HG3	1:F:2240:LEU:HD12	1.98	0.45
1:J:2168:ARG:HH12	1:K:3162:ASN:HD21	1.65	0.45
1:B:2189:LEU:HD11	1:B:2200:MET:HE2	1.97	0.45
1:G:3139:GLU:OE1	1:H:4053:HIS:HE1	2.00	0.45
1:K:3013:ILE:HA	1:K:3019:LEU:HD11	1.99	0.45
1:L:4046:LYS:HG2	1:L:4056:ARG:O	2.16	0.45
1:D:4124:LYS:HD3	1:D:4152:THR:HB	1.99	0.45
1:E:1188:GLN:HE21	1:E:1190:PRO:HG3	1.82	0.45
1:F:2223:THR:HG21	1:F:2243:LEU:HD21	1.98	0.45
1:K:3106:ARG:HB2	4:K:6017:HOH:O	2.17	0.45
1:B:2004:PHE:CE1	1:B:2250:ILE:HD12	2.52	0.45
1:F:2168:ARG:HH12	1:G:3162:ASN:HD21	1.64	0.45
1:H:4184:THR:HG23	1:H:4221:MET:HA	1.99	0.45
1:I:1150:TYR:CE2	1:I:1178:LYS:HD2	2.52	0.45
1:J:2026:ILE:HD12	1:J:2040:PHE:HD1	1.82	0.45
1:C:3119:ARG:HG2	1:C:3119:ARG:HH11	1.81	0.44
1:D:4184:THR:HG21	1:D:4222:GLU:N	2.27	0.44
1:F:2189:LEU:HD21	1:F:2200:MET:HE3	1.99	0.44
1:F:2256:VAL:HG11	1:G:3252:GLU:HB3	1.99	0.44
1:K:3008:ALA:HA	1:K:3221:MET:O	2.17	0.44
1:C:3041:LYS:HB2	1:C:3079:THR:CG2	2.47	0.44
1:H:4221:MET:CE	1:H:4238:LEU:HD23	2.47	0.44
1:A:1182:ASP:HA	1:A:1220:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2227:PRO:HB3	1:F:2237:ALA:HB3	1.99	0.44
1:F:2263:THR:HG22	1:F:2264:ILE:N	2.32	0.44
1:G:3242:GLN:O	1:G:3246:ILE:HG12	2.17	0.44
1:I:1048:ASN:N	1:I:1048:ASN:ND2	2.64	0.44
1:C:3239:PRO:HG2	1:C:3242:GLN:HE21	1.81	0.44
1:D:4097:ILE:HG12	1:D:4120:ALA:HB3	1.99	0.44
1:D:4182:ASP:HA	1:D:4220:PHE:HB3	1.99	0.44
1:E:1212:VAL:HG11	1:E:1250:ILE:HB	1.99	0.44
1:G:3019:LEU:HD22	1:G:3066:ALA:HB1	2.00	0.44
1:H:4188:GLN:HA	1:H:4199:GLY:HA2	1.99	0.44
1:L:4220:PHE:CD1	1:L:4220:PHE:C	2.91	0.44
1:A:1089:GLU:HG3	4:A:6069:HOH:O	2.17	0.44
1:B:2250:ILE:HG13	1:B:2251:LEU:N	2.33	0.44
1:E:1026:ILE:HD12	1:E:1040:PHE:CD1	2.52	0.44
1:G:3201:ARG:HG3	1:G:3204:ILE:HD12	1.98	0.44
1:K:3045:ASP:OD1	1:K:3056:ARG:HB3	2.18	0.44
1:F:2162:ASN:HD21	1:G:3168:ARG:HH12	1.64	0.44
1:I:1242:GLN:O	1:I:1246:ILE:HG12	2.17	0.44
1:J:2003:LYS:N	4:J:5093:HOH:O	2.51	0.44
1:L:4005:LEU:HD11	1:L:4039:VAL:HG23	2.00	0.44
1:L:4011:ASN:ND2	1:L:4232:SER:HB3	2.29	0.44
1:C:3097:ILE:HG12	1:C:3120:ALA:HB3	2.00	0.44
1:C:3192:GLY:C	1:C:3193:LEU:HD12	2.38	0.44
1:G:3189:LEU:HD21	1:G:3200:MET:HE2	1.99	0.44
1:C:3008:ALA:HA	1:C:3221:MET:O	2.17	0.44
1:C:3242:GLN:O	1:C:3246:ILE:HG12	2.17	0.44
1:D:4225:PRO:HG3	1:D:4240:LEU:HD12	1.99	0.44
1:F:2003:LYS:HB2	1:F:2035:GLU:O	2.18	0.44
1:F:2263:THR:O	1:F:2264:ILE:OXT	2.36	0.44
1:H:4011:ASN:HD21	1:H:4046:LYS:CE	2.31	0.44
1:B:2263:THR:O	1:B:2264:ILE:OXT	2.36	0.43
1:C:3003:LYS:HD2	1:C:3035:GLU:O	2.18	0.43
1:G:3074:PHE:O	1:G:3076:LEU:HD13	2.18	0.43
1:I:1050:SER:O	1:J:2136:ASN:HB3	2.18	0.43
1:B:2258:SER:HA	1:B:2261:TYR:CE2	2.53	0.43
1:C:3011:ASN:HD21	1:C:3046:LYS:NZ	2.16	0.43
1:C:3129:LEU:HG	1:C:3133:ASP:HB2	2.00	0.43
1:E:1168:ARG:HH12	1:H:4162:ASN:HD21	1.65	0.43
1:J:2040:PHE:HB3	1:J:2078:ILE:HD13	2.00	0.43
1:C:3052:ILE:HG23	1:C:3053:HIS:CD2	2.52	0.43
1:F:2013:ILE:HD12	1:F:2044:PHE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3184:THR:CG2	1:G:3222:GLU:H	2.28	0.43
1:D:4221:MET:HE3	1:D:4238:LEU:HD22	2.01	0.43
1:B:2041:LYS:HD3	1:B:2041:LYS:C	2.38	0.43
1:C:3026:ILE:HD12	1:C:3040:PHE:CD1	2.54	0.43
1:E:1004:PHE:HE1	1:E:1219:VAL:HG22	1.83	0.43
1:F:2036:VAL:HG22	1:F:2251:LEU:HD21	1.99	0.43
1:G:3113:ALA:HA	1:G:3116:LYS:HG2	2.00	0.43
1:H:4005:LEU:HD11	1:H:4039:VAL:CG2	2.48	0.43
1:I:1174:LYS:HG3	1:I:1264:ILE:HD13	2.00	0.43
1:I:1048:ASN:O	1:J:2106:ARG:NH1	2.51	0.43
1:J:2064:VAL:HG13	1:J:2094:VAL:CG2	2.49	0.43
1:J:2189:LEU:HD21	1:J:2200:MET:HE2	2.00	0.43
1:K:3174:LYS:CG	1:K:3264:ILE:HG21	2.43	0.43
1:K:3223:THR:OG1	1:K:3240:LEU:HA	2.18	0.43
1:L:4190:PRO:HG3	4:L:5698:HOH:O	2.18	0.43
1:D:4193:LEU:HD23	1:D:4198:GLY:CA	2.48	0.43
1:E:1113:ALA:O	1:E:1117:THR:HG23	2.18	0.43
1:F:2036:VAL:CG2	1:F:2251:LEU:HD21	2.49	0.43
1:F:2094:VAL:O	1:F:2094:VAL:HG12	2.19	0.43
1:B:2234:ALA:HA	4:B:5271:HOH:O	2.19	0.43
1:C:3174:LYS:CG	1:C:3264:ILE:HD13	2.36	0.43
1:H:4044:PHE:CZ	1:H:4060:LEU:HD13	2.53	0.43
1:J:2003:LYS:HB2	1:J:2035:GLU:O	2.19	0.43
1:J:2064:VAL:HG13	1:J:2094:VAL:HG21	2.01	0.43
1:L:4047:ALA:HB3	1:L:4083:HIS:CD2	2.54	0.43
1:J:2228:GLU:HG2	1:J:2229:LYS:HG3	2.01	0.43
1:B:2048:ASN:HD22	1:B:2048:ASN:N	2.03	0.42
1:H:4047:ALA:HB1	4:H:5148:HOH:O	2.19	0.42
1:J:2264:ILE:HG23	1:J:2264:ILE:OXT	2.19	0.42
1:K:3013:ILE:HG23	1:K:3019:LEU:CD1	2.49	0.42
1:D:4026:ILE:HD12	1:D:4040:PHE:HD1	1.83	0.42
1:D:4041:LYS:HD3	1:D:4041:LYS:C	2.40	0.42
4:E:5571:HOH:O	1:F:2047:ALA:HB1	2.18	0.42
1:G:3113:ALA:HA	1:G:3116:LYS:NZ	2.34	0.42
1:H:4019:LEU:HD12	1:H:4066:ALA:HB1	2.00	0.42
1:J:2016:GLU:O	1:J:2020:LEU:HG	2.19	0.42
1:C:3048:ASN:H	1:C:3048:ASN:HD22	1.67	0.42
1:C:3162:ASN:ND2	1:C:3163:LEU:N	2.67	0.42
1:E:1019:LEU:HD22	1:E:1066:ALA:HB1	2.00	0.42
1:F:2212:VAL:HG23	1:F:2253:ILE:CG2	2.49	0.42
1:K:3069:LYS:HE3	1:K:3073:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4154:ARG:NH2	1:L:4188:GLN:NE2	2.56	0.42
1:L:4234:ALA:N	1:L:4235:PRO:HD2	2.34	0.42
1:D:4258:SER:HA	1:D:4261:TYR:CD2	2.53	0.42
1:H:4250:ILE:HG13	1:H:4251:LEU:N	2.35	0.42
1:L:4055:PHE:CZ	1:L:4057:GLY:HA2	2.54	0.42
1:A:1183:ALA:HB2	1:A:1208:ILE:HG12	2.01	0.42
1:B:2154:ARG:O	1:B:2154:ARG:HD3	2.19	0.42
1:C:3162:ASN:HD22	1:C:3163:LEU:N	2.15	0.42
1:F:2172:ILE:HA	1:F:2175:GLN:HE21	1.84	0.42
1:I:1051:SER:HB2	1:I:1195:ASP:HB2	2.00	0.42
1:I:1235:PRO:HA	4:I:5574:HOH:O	2.18	0.42
1:K:3048:ASN:HD22	1:K:3048:ASN:H	1.68	0.42
1:K:3087:GLN:O	1:K:3091:VAL:HG23	2.19	0.42
1:A:1030:SER:HA	1:A:1038:PHE:CE1	2.55	0.42
1:F:2122:ASN:HA	1:F:2150:TYR:HB2	2.00	0.42
1:I:1016:GLU:O	1:I:1020:LEU:HG	2.20	0.42
1:I:1154:ARG:O	1:I:1154:ARG:HD3	2.20	0.42
1:J:2044:PHE:CZ	1:J:2060:LEU:HD13	2.55	0.42
1:J:2130:ALA:O	1:J:2133:ASP:HB2	2.20	0.42
1:B:2162:ASN:ND2	1:B:2163:LEU:H	2.17	0.42
1:B:2201:ARG:HH22	1:B:2227:PRO:HB2	1.85	0.42
1:G:3060:LEU:HD12	1:G:3064:VAL:HG23	2.00	0.42
1:I:1041:LYS:HD3	1:I:1041:LYS:C	2.39	0.42
1:K:3082:ILE:HG13	1:K:3110:LEU:HD11	2.02	0.42
1:C:3016:GLU:O	1:C:3020:LEU:HG	2.20	0.42
1:H:4189:LEU:HD23	4:H:6428:HOH:O	2.19	0.42
1:H:4238:LEU:HD21	1:H:4246:ILE:CD1	2.49	0.42
1:K:3097:ILE:HG12	1:K:3120:ALA:HB3	2.02	0.42
1:L:4228:GLU:HB3	4:L:6475:HOH:O	2.20	0.42
1:K:3124:LYS:HD3	1:K:3152:THR:HB	2.00	0.42
1:A:1259:LYS:HE3	1:A:1259:LYS:HB2	1.87	0.41
1:B:2264:ILE:OXT	1:B:2264:ILE:HG23	2.20	0.41
1:D:4026:ILE:HD12	1:D:4040:PHE:CD1	2.55	0.41
1:F:2213:ALA:HB2	1:G:3213:ALA:HB2	2.02	0.41
1:I:1201:ARG:NH2	1:I:1234:ALA:O	2.53	0.41
1:A:1252:GLU:OE1	1:D:4260:TYR:OH	2.33	0.41
1:E:1005:LEU:HD12	1:E:1037:GLU:O	2.19	0.41
1:E:1201:ARG:HG3	1:E:1204:ILE:HD12	2.02	0.41
1:J:2078:ILE:HG22	1:J:2079:THR:N	2.35	0.41
1:J:2201:ARG:NH2	1:J:2227:PRO:CB	2.84	0.41
1:L:4011:ASN:HD21	1:L:4046:LYS:HE2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1189:LEU:HD21	1:E:1200:MET:CE	2.51	0.41
1:F:2048:ASN:C	1:F:2048:ASN:HD22	2.22	0.41
1:G:3040:PHE:HB3	1:G:3078:ILE:HD13	2.01	0.41
1:G:3162:ASN:HD22	1:G:3163:LEU:N	2.16	0.41
1:H:4221:MET:HE3	1:H:4238:LEU:HD23	2.02	0.41
1:J:2003:LYS:N	4:J:6107:HOH:O	2.54	0.41
1:J:2136:ASN:HD22	1:J:2136:ASN:HA	1.67	0.41
1:K:3046:LYS:HB3	1:K:3049:ARG:HD3	2.02	0.41
1:L:4154:ARG:HH12	1:L:4188:GLN:NE2	2.15	0.41
1:L:4208:ILE:CD1	1:L:4219:VAL:HG11	2.50	0.41
1:B:2243:LEU:N	1:B:2243:LEU:HD12	2.35	0.41
1:C:3119:ARG:HG2	1:C:3119:ARG:NH1	2.35	0.41
1:C:3223:THR:OG1	1:C:3240:LEU:HA	2.20	0.41
1:E:1174:LYS:HG3	1:E:1264:ILE:HG21	2.02	0.41
1:F:2009:GLY:H	1:F:2223:THR:HG22	1.86	0.41
1:H:4136:ASN:HD22	1:H:4136:ASN:HA	1.63	0.41
1:D:4020:LEU:HD21	1:D:4069:LYS:HG3	2.02	0.41
1:E:1004:PHE:HZ	1:E:1219:VAL:HG13	1.86	0.41
1:E:1203:PHE:HA	1:E:1206:PRO:CG	2.51	0.41
1:I:1044:PHE:CE2	1:I:1060:LEU:HD13	2.55	0.41
1:A:1010:PRO:HA	1:A:1223:THR:O	2.20	0.41
1:D:4212:VAL:HG23	1:D:4253:ILE:CG2	2.50	0.41
1:E:1055:PHE:CZ	1:E:1057:GLY:HA2	2.55	0.41
1:H:4208:ILE:CD1	1:H:4219:VAL:HG11	2.50	0.41
1:I:1162:ASN:HD22	1:I:1163:LEU:H	1.67	0.41
1:B:2182:ASP:HA	1:B:2220:PHE:HB3	2.02	0.41
1:E:1162:ASN:HD22	1:E:1163:LEU:H	1.68	0.41
1:J:2004:PHE:CE1	1:J:2250:ILE:HD12	2.55	0.41
1:B:2011:ASN:HD21	1:B:2046:LYS:NZ	2.18	0.41
1:B:2258:SER:HA	1:B:2261:TYR:CD2	2.56	0.41
1:I:1055:PHE:CZ	1:I:1057:GLY:HA2	2.55	0.41
1:I:1250:ILE:HG13	1:I:1251:LEU:N	2.36	0.41
1:C:3174:LYS:HG3	1:C:3264:ILE:HG21	2.02	0.41
1:C:3174:LYS:HE3	1:C:3264:ILE:CD1	2.51	0.41
1:D:4128:PHE:HB3	4:D:5182:HOH:O	2.20	0.41
1:E:1041:LYS:HD3	1:E:1041:LYS:C	2.41	0.41
1:F:2048:ASN:C	1:F:2048:ASN:ND2	2.73	0.41
1:F:2071:LYS:O	1:F:2075:GLY:N	2.52	0.41
1:F:2188:GLN:HB3	1:F:2236:THR:HG21	2.01	0.41
1:G:3008:ALA:HA	1:G:3221:MET:O	2.20	0.41
1:H:4044:PHE:CE2	1:H:4060:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2094:VAL:HA	4:J:6481:HOH:O	2.21	0.41
1:K:3157:THR:HG23	4:K:6096:HOH:O	2.19	0.41
1:L:4078:ILE:HG22	1:L:4079:THR:N	2.35	0.41
1:L:4138:VAL:CG1	1:L:4142:LYS:HE3	2.51	0.41
1:B:2021:LYS:HE3	1:B:2225:PRO:HB3	2.02	0.41
1:D:4192:GLY:C	1:D:4193:LEU:HD22	2.41	0.41
1:E:1019:LEU:HD12	1:E:1019:LEU:N	2.36	0.41
1:F:2068:ARG:N	1:F:2094:VAL:HG11	2.36	0.41
1:G:3243:LEU:O	1:G:3247:ILE:HG13	2.21	0.41
1:H:4258:SER:HA	1:H:4261:TYR:CD2	2.55	0.41
1:J:2263:THR:O	1:J:2264:ILE:OXT	2.39	0.41
1:K:3048:ASN:HD22	1:K:3048:ASN:C	2.24	0.41
1:K:3141:LEU:O	1:K:3146:ALA:HB3	2.20	0.41
1:L:4011:ASN:HD21	1:L:4046:LYS:NZ	2.19	0.41
1:L:4013:ILE:HG23	1:L:4019:LEU:HD11	2.03	0.41
1:L:4016:GLU:HG2	1:L:4020:LEU:CD1	2.50	0.41
1:E:1050:SER:O	1:F:2136:ASN:HB3	2.21	0.40
1:F:2187:VAL:HG21	1:F:2204:ILE:HG12	2.02	0.40
1:B:2136:ASN:HD22	1:B:2136:ASN:HA	1.67	0.40
1:J:2252:GLU:HB3	1:K:3256:VAL:HG21	2.03	0.40
1:K:3089:GLU:HB3	1:K:3090:PRO:CD	2.51	0.40
1:D:4051:SER:HB2	1:D:4195:ASP:HB2	2.04	0.40
1:F:2004:PHE:HZ	1:F:2219:VAL:HG23	1.85	0.40
1:K:3148:GLU:HG2	1:K:3150:TYR:CE1	2.57	0.40
1:K:3185:HIS:O	1:K:3188:GLN:HG2	2.21	0.40
1:K:3205:PHE:N	1:K:3206:PRO:HD2	2.36	0.40
1:L:4148:GLU:HG2	1:L:4150:TYR:CE1	2.55	0.40
1:A:1139:GLU:OE1	1:B:2053:HIS:HE1	2.03	0.40
1:A:1154:ARG:NH2	1:A:1188:GLN:NE2	2.57	0.40
1:C:3025:GLU:HA	1:C:3025:GLU:OE1	2.20	0.40
1:F:2238:LEU:HD12	1:F:2239:PRO:CD	2.49	0.40
1:I:1010:PRO:HA	1:I:1223:THR:O	2.22	0.40
1:L:4162:ASN:ND2	1:L:4163:LEU:N	2.69	0.40
1:B:2013:ILE:HD12	1:B:2044:PHE:HA	2.04	0.40
1:B:2159:GLY:HA3	1:D:4159:GLY:HA3	2.04	0.40
1:E:1004:PHE:CE1	1:E:1250:ILE:HD12	2.55	0.40
1:G:3026:ILE:HD12	1:G:3040:PHE:CD1	2.57	0.40
1:G:3077:LYS:NZ	4:G:5727:HOH:O	2.55	0.40
1:K:3188:GLN:HA	1:K:3199:GLY:HA2	2.02	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	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
1	B	260/263 (99%)	251 (96%)	8 (3%)	1 (0%)	34	32
1	C	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
1	D	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
1	E	255/263 (97%)	234 (92%)	21 (8%)	0	100	100
1	F	260/263 (99%)	239 (92%)	20 (8%)	1 (0%)	34	32
1	G	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
1	H	252/263 (96%)	247 (98%)	5 (2%)	0	100	100
1	I	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
1	J	251/263 (95%)	243 (97%)	8 (3%)	0	100	100
1	K	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
1	L	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
All	All	3098/3156 (98%)	2962 (96%)	134 (4%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	2092	ALA
1	B	2235	PRO

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	218/219 (100%)	209 (96%)	9 (4%)	30	30
1	B	218/219 (100%)	211 (97%)	7 (3%)	39	40
1	C	218/219 (100%)	213 (98%)	5 (2%)	50	53
1	D	218/219 (100%)	213 (98%)	5 (2%)	50	53
1	E	216/219 (99%)	212 (98%)	4 (2%)	57	61
1	F	218/219 (100%)	212 (97%)	6 (3%)	43	46
1	G	218/219 (100%)	212 (97%)	6 (3%)	43	46
1	H	214/219 (98%)	208 (97%)	6 (3%)	43	46
1	I	218/219 (100%)	213 (98%)	5 (2%)	50	53
1	J	214/219 (98%)	208 (97%)	6 (3%)	43	46
1	K	218/219 (100%)	214 (98%)	4 (2%)	59	63
1	L	218/219 (100%)	212 (97%)	6 (3%)	43	46
All	All	2606/2628 (99%)	2537 (97%)	69 (3%)	46	49

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	ASN
1	A	1106	ARG
1	A	1112	LEU
1	A	1154	ARG
1	A	1162	ASN
1	A	1176	TRP
1	A	1184	THR
1	A	1228	GLU
1	A	1243	LEU
1	B	2016	GLU
1	B	2029	LEU
1	B	2035	GLU
1	B	2048	ASN
1	B	2154	ARG
1	B	2162	ASN
1	B	2228	GLU
1	C	3048	ASN
1	C	3112	LEU
1	C	3154	ARG
1	C	3162	ASN
1	C	3250	ILE
1	D	4029	LEU

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Mol	Chain	Res	Type
1	D	4048	ASN
1	D	4154	ARG
1	D	4162	ASN
1	D	4176	TRP
1	E	1048	ASN
1	E	1154	ARG
1	E	1176	TRP
1	E	1226	GLU
1	F	2016	GLU
1	F	2048	ASN
1	F	2122	ASN
1	F	2154	ARG
1	F	2162	ASN
1	F	2176	TRP
1	G	3048	ASN
1	G	3154	ARG
1	G	3162	ASN
1	G	3176	TRP
1	G	3228	GLU
1	G	3243	LEU
1	H	4048	ASN
1	H	4106	ARG
1	H	4154	ARG
1	H	4162	ASN
1	H	4176	TRP
1	H	4188	GLN
1	I	1048	ASN
1	I	1076	LEU
1	I	1112	LEU
1	I	1154	ARG
1	I	1162	ASN
1	J	2048	ASN
1	J	2106	ARG
1	J	2147	LYS
1	J	2154	ARG
1	J	2162	ASN
1	J	2240	LEU
1	K	3048	ASN
1	K	3154	ARG
1	K	3162	ASN
1	K	3176	TRP
1	L	4069	LYS

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Mol	Chain	Res	Type
1	L	4154	ARG
1	L	4162	ASN
1	L	4176	TRP
1	L	4220	PHE
1	L	4240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	ASN
1	A	1048	ASN
1	A	1058	HIS
1	A	1099	GLN
1	A	1136	ASN
1	A	1161	ASN
1	A	1162	ASN
1	A	1175	GLN
1	A	1188	GLN
1	A	1242	GLN
1	B	2011	ASN
1	B	2048	ASN
1	B	2053	HIS
1	B	2058	HIS
1	B	2122	ASN
1	B	2161	ASN
1	B	2162	ASN
1	B	2188	GLN
1	C	3011	ASN
1	C	3048	ASN
1	C	3053	HIS
1	C	3058	HIS
1	C	3099	GLN
1	C	3161	ASN
1	C	3162	ASN
1	C	3188	GLN
1	C	3242	GLN
1	D	4048	ASN
1	D	4053	HIS
1	D	4058	HIS
1	D	4083	HIS
1	D	4107	GLN
1	D	4122	ASN

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Mol	Chain	Res	Type
1	D	4136	ASN
1	D	4161	ASN
1	D	4162	ASN
1	E	1011	ASN
1	E	1048	ASN
1	E	1053	HIS
1	E	1099	GLN
1	E	1136	ASN
1	E	1161	ASN
1	E	1162	ASN
1	E	1175	GLN
1	E	1188	GLN
1	E	1242	GLN
1	F	2048	ASN
1	F	2058	HIS
1	F	2099	GLN
1	F	2107	GLN
1	F	2122	ASN
1	F	2136	ASN
1	F	2161	ASN
1	F	2162	ASN
1	F	2175	GLN
1	F	2188	GLN
1	F	2242	GLN
1	G	3011	ASN
1	G	3048	ASN
1	G	3053	HIS
1	G	3058	HIS
1	G	3161	ASN
1	G	3162	ASN
1	G	3188	GLN
1	H	4011	ASN
1	H	4048	ASN
1	H	4058	HIS
1	H	4099	GLN
1	H	4122	ASN
1	H	4136	ASN
1	H	4161	ASN
1	H	4162	ASN
1	H	4188	GLN
1	I	1011	ASN
1	I	1048	ASN

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Mol	Chain	Res	Type
1	I	1058	HIS
1	I	1099	GLN
1	I	1161	ASN
1	I	1162	ASN
1	I	1188	GLN
1	J	2011	ASN
1	J	2048	ASN
1	J	2058	HIS
1	J	2083	HIS
1	J	2122	ASN
1	J	2161	ASN
1	J	2162	ASN
1	J	2188	GLN
1	J	2242	GLN
1	K	3011	ASN
1	K	3048	ASN
1	K	3053	HIS
1	K	3136	ASN
1	K	3161	ASN
1	K	3162	ASN
1	K	3175	GLN
1	K	3242	GLN
1	L	4011	ASN
1	L	4058	HIS
1	L	4099	GLN
1	L	4122	ASN
1	L	4161	ASN
1	L	4162	ASN
1	L	4188	GLN

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)

24 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	$\#\|Z\| > 2$
2	PO4	A	1280	-	4,4,4	1.61	1 (25%)	6,6,6	0.43	0
2	PO4	H	1287	-	4,4,4	1.59	0	6,6,6	0.43	0
3	PEP	H	1275	-	9,9,9	0.95	0	11,13,13	1.27	2 (18%)
3	PEP	E	1272	-	9,9,9	1.11	0	11,13,13	1.68	2 (18%)
3	PEP	A	1268	-	9,9,9	0.88	0	11,13,13	1.56	1 (9%)
3	PEP	I	1276	-	9,9,9	0.87	0	11,13,13	1.28	1 (9%)
2	PO4	I	1288	-	4,4,4	1.62	0	6,6,6	0.44	0
2	PO4	J	1289	-	4,4,4	1.66	0	6,6,6	0.42	0
3	PEP	D	1271	-	9,9,9	0.98	0	11,13,13	1.71	2 (18%)
3	PEP	B	1269	-	9,9,9	1.08	1 (11%)	11,13,13	1.58	2 (18%)
3	PEP	G	1274	-	9,9,9	1.09	1 (11%)	11,13,13	1.60	1 (9%)
2	PO4	K	1290	-	4,4,4	1.69	0	6,6,6	0.45	0
3	PEP	F	1273	-	9,9,9	1.15	0	11,13,13	1.52	2 (18%)
2	PO4	C	1282	-	4,4,4	1.65	0	6,6,6	0.44	0
2	PO4	L	1291	-	4,4,4	1.62	0	6,6,6	0.44	0
3	PEP	J	1277	-	9,9,9	0.84	0	11,13,13	1.48	3 (27%)
2	PO4	G	1286	-	4,4,4	1.59	0	6,6,6	0.45	0
2	PO4	F	1285	-	4,4,4	1.64	0	6,6,6	0.44	0
2	PO4	B	1281	-	4,4,4	1.63	0	6,6,6	0.43	0
2	PO4	E	1284	-	4,4,4	1.64	0	6,6,6	0.44	0
3	PEP	C	1270	-	9,9,9	1.16	0	11,13,13	1.65	2 (18%)
2	PO4	D	1283	-	4,4,4	1.65	0	6,6,6	0.45	0
3	PEP	L	1279	-	9,9,9	1.09	0	11,13,13	1.49	2 (18%)
3	PEP	K	1278	-	9,9,9	1.13	0	11,13,13	1.40	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEP	L	1279	-	-	0/9/9/9	-
3	PEP	J	1277	-	-	0/9/9/9	-
3	PEP	H	1275	-	-	0/9/9/9	-
3	PEP	D	1271	-	-	0/9/9/9	-
3	PEP	E	1272	-	-	1/9/9/9	-
3	PEP	B	1269	-	-	0/9/9/9	-
3	PEP	G	1274	-	-	0/9/9/9	-
3	PEP	C	1270	-	-	0/9/9/9	-
3	PEP	F	1273	-	-	0/9/9/9	-
3	PEP	A	1268	-	-	0/9/9/9	-
3	PEP	K	1278	-	-	4/9/9/9	-
3	PEP	I	1276	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1269	PEP	P-O2	2.21	1.62	1.59
2	A	1280	PO4	P-O3	-2.00	1.48	1.54
3	G	1274	PEP	P-O2	2.00	1.62	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1271	PEP	O2'-C1-C2	4.37	121.37	113.91
3	G	1274	PEP	O2'-C1-C2	4.32	121.27	113.91
3	C	1270	PEP	O2'-C1-C2	4.30	121.25	113.91
3	B	1269	PEP	O2'-C1-C2	4.07	120.85	113.91
3	A	1268	PEP	O2'-C1-C2	3.71	120.23	113.91
3	F	1273	PEP	O2'-C1-C2	3.60	120.05	113.91
3	J	1277	PEP	O2'-C1-C2	3.44	119.78	113.91
3	H	1275	PEP	O2'-C1-C2	3.43	119.76	113.91
3	K	1278	PEP	O2'-C1-C2	3.34	119.60	113.91
3	E	1272	PEP	O2'-C1-C2	3.19	119.35	113.91
3	L	1279	PEP	O2'-C1-C2	3.14	119.27	113.91
3	I	1276	PEP	O2'-C1-C2	2.94	118.93	113.91
3	E	1272	PEP	O2'-C1-O1	-2.92	116.92	123.61
3	F	1273	PEP	O2'-C1-O1	-2.87	117.03	123.61
3	L	1279	PEP	O2'-C1-O1	-2.60	117.65	123.61
3	D	1271	PEP	O2'-C1-O1	-2.58	117.71	123.61
3	K	1278	PEP	O2'-C1-O1	-2.56	117.75	123.61
3	C	1270	PEP	O2'-C1-O1	-2.48	117.93	123.61
3	J	1277	PEP	O3P-P-O1P	2.38	119.98	110.68
3	B	1269	PEP	O2'-C1-O1	-2.23	118.50	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1275	PEP	O2'-C1-O1	-2.08	118.84	123.61
3	J	1277	PEP	O2'-C1-O1	-2.02	118.98	123.61

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1272	PEP	C2-O2-P-O1P
3	K	1278	PEP	O2'-C1-C2-C3
3	K	1278	PEP	O2'-C1-C2-O2
3	K	1278	PEP	O1-C1-C2-O2
3	K	1278	PEP	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	262/263 (99%)	0.21	13 (4%)	28	34	15, 24, 46, 69	0
1	B	262/263 (99%)	0.37	15 (5%)	23	28	13, 24, 47, 78	0
1	C	262/263 (99%)	0.56	19 (7%)	15	19	19, 41, 57, 67	0
1	D	262/263 (99%)	0.96	31 (11%)	4	5	21, 44, 65, 79	0
1	E	259/263 (98%)	1.08	47 (18%)	1	1	23, 52, 71, 79	0
1	F	262/263 (99%)	1.58	71 (27%)	0	0	25, 57, 75, 83	0
1	G	262/263 (99%)	0.38	17 (6%)	18	23	17, 29, 59, 77	0
1	H	256/263 (97%)	0.20	8 (3%)	49	55	15, 26, 47, 79	0
1	I	262/263 (99%)	0.31	15 (5%)	23	28	15, 25, 47, 73	0
1	J	255/263 (96%)	0.20	7 (2%)	54	60	14, 27, 49, 75	0
1	K	262/263 (99%)	1.36	63 (24%)	0	0	26, 56, 73, 77	0
1	L	262/263 (99%)	0.85	29 (11%)	5	6	22, 45, 62, 79	0
All	All	3128/3156 (99%)	0.67	335 (10%)	6	7	13, 36, 68, 83	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2193	LEU	11.4
1	G	3264	ILE	10.0
1	F	2264	ILE	9.5
1	H	4264	ILE	9.4
1	I	1193	LEU	9.0
1	J	2264	ILE	8.8
1	B	2194	GLY	8.2
1	B	2197	SER	8.1
1	D	4264	ILE	8.0
1	L	4264	ILE	8.0
1	B	2264	ILE	7.7

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Mol	Chain	Res	Type	RSRZ
1	D	4193	LEU	7.3
1	I	1197	SER	7.0
1	L	4195	ASP	7.0
1	K	3264	ILE	6.9
1	L	4193	LEU	6.9
1	F	2197	SER	6.8
1	G	3193	LEU	6.6
1	F	2263	THR	6.5
1	K	3193	LEU	6.5
1	F	2057	GLY	6.5
1	D	4263	THR	6.4
1	A	1195	ASP	6.4
1	C	3193	LEU	6.4
1	B	2193	LEU	6.3
1	G	3263	THR	6.0
1	G	3194	GLY	6.0
1	I	1194	GLY	5.9
1	H	4263	THR	5.9
1	B	2198	GLY	5.9
1	K	3063	GLY	5.9
1	K	3198	GLY	5.9
1	D	4197	SER	5.9
1	I	1264	ILE	5.8
1	E	1198	GLY	5.8
1	L	4198	GLY	5.7
1	D	4198	GLY	5.6
1	F	2220	PHE	5.6
1	B	2196	LYS	5.6
1	D	4196	LYS	5.6
1	E	1193	LEU	5.6
1	K	3076	LEU	5.5
1	F	2195	ASP	5.5
1	K	3057	GLY	5.5
1	E	1197	SER	5.4
1	E	1231	LEU	5.4
1	F	2194	GLY	5.4
1	A	1193	LEU	5.3
1	B	2195	ASP	5.3
1	E	1016	GLU	5.3
1	F	2196	LYS	5.2
1	K	3195	ASP	5.2
1	A	1264	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	K	3197	SER	5.1
1	K	3192	GLY	5.1
1	J	2263	THR	5.1
1	I	1263	THR	5.0
1	G	3192	GLY	5.0
1	I	1192	GLY	5.0
1	L	4196	LYS	5.0
1	F	2192	GLY	5.0
1	L	4235	PRO	5.0
1	F	2198	GLY	4.9
1	E	1147	LYS	4.9
1	G	3198	GLY	4.9
1	I	1198	GLY	4.9
1	K	3200	MET	4.9
1	F	2094	VAL	4.9
1	G	3195	ASP	4.8
1	F	2007	ILE	4.8
1	K	3196	LYS	4.7
1	E	1061	GLU	4.6
1	D	4195	ASP	4.6
1	K	3194	GLY	4.5
1	F	2068	ARG	4.4
1	K	3235	PRO	4.4
1	F	2141	LEU	4.4
1	B	2192	GLY	4.4
1	F	2228	GLU	4.4
1	A	1194	GLY	4.3
1	H	4235	PRO	4.3
1	J	2235	PRO	4.3
1	C	3264	ILE	4.3
1	K	3220	PHE	4.2
1	E	1075	GLY	4.2
1	E	1220	PHE	4.2
1	F	2070	VAL	4.2
1	C	3195	ASP	4.2
1	B	2263	THR	4.1
1	K	3263	THR	4.1
1	F	2035	GLU	4.1
1	L	4197	SER	4.1
1	F	2219	VAL	4.0
1	L	4194	GLY	3.9
1	K	3086	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	1199	GLY	3.9
1	F	2074	PHE	3.9
1	G	3197	SER	3.8
1	K	3036	VAL	3.8
1	F	2235	PRO	3.7
1	A	1192	GLY	3.7
1	E	1007	ILE	3.7
1	F	2072	GLU	3.7
1	D	4072	GLU	3.7
1	A	1263	THR	3.7
1	K	3116	LYS	3.6
1	H	4198	GLY	3.6
1	E	1065	LYS	3.6
1	J	2200	MET	3.6
1	C	3194	GLY	3.5
1	L	4116	LYS	3.5
1	B	2235	PRO	3.5
1	E	1052	ILE	3.5
1	F	2227	PRO	3.5
1	K	3241	SER	3.5
1	K	3018	LEU	3.5
1	E	1191	GLY	3.5
1	C	3235	PRO	3.4
1	E	1143	PHE	3.4
1	E	1146	ALA	3.4
1	B	2191	GLY	3.4
1	F	2006	VAL	3.4
1	G	3196	LYS	3.4
1	E	1226	GLU	3.3
1	K	3020	LEU	3.3
1	K	3231	LEU	3.3
1	D	4069	LYS	3.3
1	F	2250	ILE	3.3
1	L	4192	GLY	3.3
1	L	4220	PHE	3.3
1	K	3007	ILE	3.3
1	K	3073	GLU	3.2
1	I	1235	PRO	3.2
1	I	1195	ASP	3.2
1	K	3069	LYS	3.2
1	E	1219	VAL	3.2
1	F	2199	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	3226	GLU	3.2
1	D	4016	GLU	3.1
1	K	3074	PHE	3.1
1	F	2146	ALA	3.1
1	G	3260	TYR	3.1
1	E	1006	VAL	3.1
1	E	1057	GLY	3.1
1	E	1263	THR	3.1
1	E	1017	GLU	3.1
1	L	4228	GLU	3.1
1	E	1020	LEU	3.1
1	K	3061	GLU	3.1
1	D	4035	GLU	3.0
1	L	4263	THR	3.0
1	C	3020	LEU	3.0
1	C	3093	GLU	3.0
1	E	1008	ALA	3.0
1	E	1232	SER	3.0
1	F	2076	LEU	3.0
1	C	3220	PHE	3.0
1	F	2226	GLU	3.0
1	D	4228	GLU	3.0
1	F	2093	GLU	3.0
1	F	2100	ILE	3.0
1	F	2069	LYS	3.0
1	I	1196	LYS	3.0
1	E	1227	PRO	3.0
1	F	2183	ALA	3.0
1	E	1118	GLY	2.9
1	K	3065	LYS	2.9
1	F	2020	LEU	2.9
1	C	3143	PHE	2.9
1	F	2018	LEU	2.9
1	L	4191	GLY	2.9
1	D	4220	PHE	2.9
1	D	4065	LYS	2.9
1	K	3034	LYS	2.9
1	K	3072	GLU	2.9
1	L	4094	VAL	2.8
1	A	1197	SER	2.8
1	E	1076	LEU	2.8
1	F	2132	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	1091	VAL	2.8
1	F	2016	GLU	2.8
1	D	4200	MET	2.8
1	K	3118	GLY	2.8
1	E	1145	GLY	2.8
1	B	2020	LEU	2.8
1	C	3116	LYS	2.8
1	D	4070	VAL	2.8
1	H	4016	GLU	2.8
1	K	3232	SER	2.8
1	E	1234	ALA	2.7
1	K	3091	VAL	2.7
1	K	3060	LEU	2.7
1	K	3089	GLU	2.7
1	K	3219	VAL	2.7
1	L	4226	GLU	2.7
1	K	3035	GLU	2.7
1	L	4034	LYS	2.7
1	L	4020	LEU	2.7
1	D	4094	VAL	2.7
1	E	1264	ILE	2.7
1	F	2176	TRP	2.7
1	F	2251	LEU	2.7
1	D	4007	ILE	2.7
1	A	1191	GLY	2.7
1	G	3176	TRP	2.6
1	K	3006	VAL	2.6
1	E	1192	GLY	2.6
1	J	2190	PRO	2.6
1	F	2249	ALA	2.6
1	E	1184	THR	2.6
1	E	1055	PHE	2.6
1	F	2143	PHE	2.6
1	D	4194	GLY	2.6
1	J	2228	GLU	2.6
1	C	3052	ILE	2.6
1	F	2061	GLU	2.6
1	H	4199	GLY	2.6
1	K	3026	ILE	2.6
1	F	2060	LEU	2.6
1	G	3251	LEU	2.6
1	D	4068	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	1241	SER	2.6
1	E	1053	HIS	2.6
1	E	1221	MET	2.6
1	F	2255	GLU	2.6
1	L	4093	GLU	2.6
1	D	4076	LEU	2.6
1	E	1060	LEU	2.6
1	C	3147	LYS	2.5
1	D	4183	ALA	2.5
1	E	1047	ALA	2.5
1	F	2029	LEU	2.5
1	F	2221	MET	2.5
1	D	4145	GLY	2.5
1	G	3259	LYS	2.5
1	K	3183	ALA	2.5
1	B	2219	VAL	2.5
1	C	3219	VAL	2.5
1	K	3191	GLY	2.5
1	F	2022	VAL	2.5
1	K	3008	ALA	2.5
1	K	3019	LEU	2.5
1	L	4114	ALA	2.5
1	C	3196	LYS	2.5
1	D	4227	PRO	2.5
1	K	3016	GLU	2.5
1	L	4143	PHE	2.5
1	K	3221	MET	2.4
1	F	2055	PHE	2.4
1	F	2152	THR	2.4
1	L	4029	LEU	2.4
1	K	3145	GLY	2.4
1	F	2181	TYR	2.4
1	A	1183	ALA	2.4
1	B	2200	MET	2.4
1	F	2053	HIS	2.4
1	D	4143	PHE	2.4
1	E	1054	SER	2.4
1	J	2191	GLY	2.4
1	F	2147	LYS	2.4
1	K	3143	PHE	2.4
1	K	3138	VAL	2.4
1	G	3200	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	4093	GLU	2.3
1	D	4116	LYS	2.3
1	F	2121	VAL	2.3
1	F	2073	GLU	2.3
1	K	3024	GLU	2.3
1	L	4123	VAL	2.3
1	K	3190	PRO	2.3
1	E	1116	LYS	2.3
1	K	3062	TYR	2.3
1	F	2248	GLU	2.3
1	L	4089	GLU	2.3
1	A	1198	GLY	2.3
1	E	1119	ARG	2.3
1	H	4191	GLY	2.3
1	I	1191	GLY	2.3
1	A	1228	GLU	2.3
1	K	3017	GLU	2.3
1	L	4200	MET	2.2
1	H	4061	GLU	2.2
1	C	3007	ILE	2.2
1	K	3052	ILE	2.2
1	F	2005	LEU	2.2
1	F	2095	ALA	2.2
1	L	4079	THR	2.2
1	B	2199	GLY	2.2
1	K	3132	TRP	2.2
1	F	2175	GLN	2.2
1	K	3181	TYR	2.2
1	K	3093	GLU	2.2
1	K	3176	TRP	2.2
1	L	4132	TRP	2.2
1	F	2026	ILE	2.2
1	C	3057	GLY	2.2
1	A	1220	PHE	2.2
1	F	2062	TYR	2.2
1	F	2091	VAL	2.2
1	K	3117	THR	2.2
1	F	2098	ILE	2.1
1	I	1132	TRP	2.1
1	F	2039	VAL	2.1
1	F	2089	GLU	2.1
1	E	1034	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	2229	LYS	2.1
1	E	1235	PRO	2.1
1	G	3007	ILE	2.1
1	A	1196	LYS	2.1
1	E	1072	GLU	2.1
1	C	3184	THR	2.1
1	I	1184	THR	2.1
1	K	3111	LEU	2.1
1	D	4235	PRO	2.1
1	F	2090	PRO	2.1
1	F	2115	ALA	2.1
1	G	3220	PHE	2.1
1	G	3235	PRO	2.1
1	C	3053	HIS	2.1
1	D	4057	GLY	2.1
1	F	2182	ASP	2.1
1	D	4184	THR	2.1
1	F	2079	THR	2.1
1	K	3152	THR	2.1
1	F	2144	GLY	2.1
1	D	4073	GLU	2.0
1	E	1104	LEU	2.0
1	F	2097	ILE	2.0
1	K	3005	LEU	2.0
1	L	4190	PRO	2.0
1	C	3229	LYS	2.0
1	I	1180	ILE	2.0
1	E	1115	ALA	2.0
1	K	3047	ALA	2.0
1	L	4144	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	K	1290	5/5	0.88	0.14	61,61,62,62	0
2	PO4	L	1291	5/5	0.89	0.15	60,60,61,61	0
2	PO4	D	1283	5/5	0.91	0.12	57,58,60,61	0
2	PO4	F	1285	5/5	0.92	0.14	62,63,64,64	0
2	PO4	E	1284	5/5	0.93	0.15	70,70,71,71	0
2	PO4	C	1282	5/5	0.93	0.10	47,50,51,51	0
2	PO4	B	1281	5/5	0.95	0.10	32,36,38,38	0
2	PO4	G	1286	5/5	0.96	0.10	35,37,39,39	0
3	PEP	F	1273	10/10	0.96	0.14	40,46,48,48	0
3	PEP	K	1278	10/10	0.96	0.18	40,45,49,50	0
2	PO4	I	1288	5/5	0.97	0.10	33,35,37,38	0
3	PEP	C	1270	10/10	0.97	0.16	28,35,37,39	0
3	PEP	D	1271	10/10	0.97	0.20	29,35,40,42	0
3	PEP	E	1272	10/10	0.97	0.18	42,46,50,50	0
2	PO4	J	1289	5/5	0.97	0.10	38,40,42,43	0
2	PO4	A	1280	5/5	0.97	0.08	31,33,35,37	0
3	PEP	G	1274	10/10	0.98	0.16	18,23,25,26	0
3	PEP	J	1277	10/10	0.98	0.18	16,20,22,22	0
2	PO4	H	1287	5/5	0.98	0.07	37,39,40,41	0
3	PEP	L	1279	10/10	0.98	0.11	32,37,41,43	0
3	PEP	I	1276	10/10	0.99	0.23	17,21,22,23	0
3	PEP	B	1269	10/10	0.99	0.18	14,17,22,26	0
3	PEP	A	1268	10/10	0.99	0.17	15,19,23,23	0
3	PEP	H	1275	10/10	0.99	0.16	15,21,23,24	0

6.5 Other polymers (i)

There are no such residues in this entry.