



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:07 PM UTC

PDB ID : 2NXH / pdb_00002nxh
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

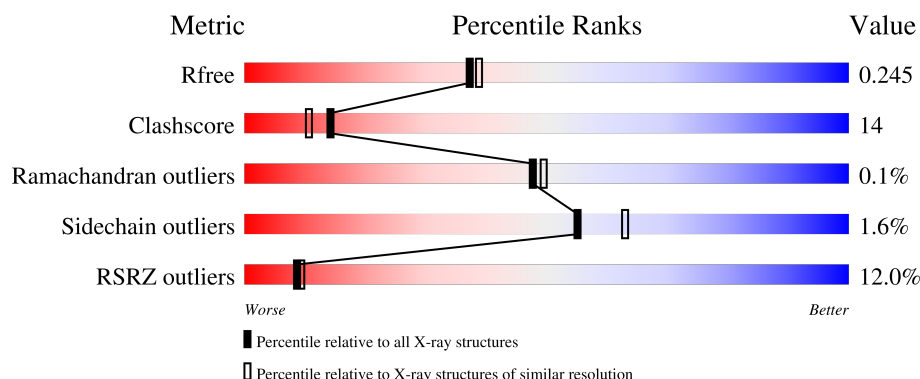
1 Overall quality at a glance

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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	5% 79% 20% .
1	B	263	6% 78% 21% .
1	C	263	8% 73% 26% .
1	D	263	12% 69% 30% .
1	E	263	22% 65% 33% .

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Mol	Chain	Length	Quality of chain
1	F	263	
1	G	263	
1	H	263	
1	I	263	
1	J	263	
1	K	263	
1	L	263	

2 Entry composition

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

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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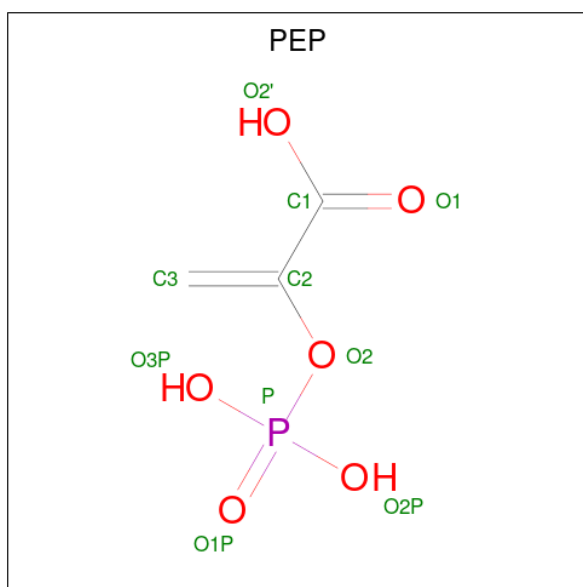
Chain	Residue	Modelled	Actual	Comment	Reference
B	2237	ALA	GLN	engineered mutation	UNP O66496
C	3011	ASN	CYS	engineered mutation	UNP O66496
C	3235	PRO	SER	engineered mutation	UNP O66496
C	3237	ALA	GLN	engineered mutation	UNP O66496
D	4011	ASN	CYS	engineered mutation	UNP O66496
D	4235	PRO	SER	engineered 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 (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



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

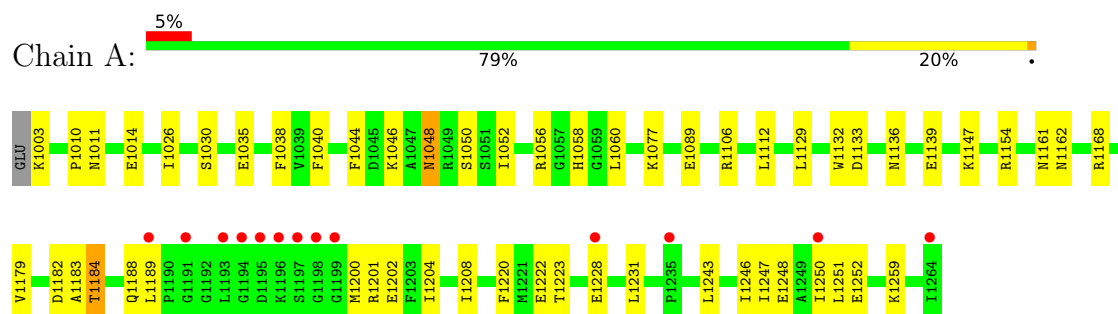
- Molecule 4 is water.

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

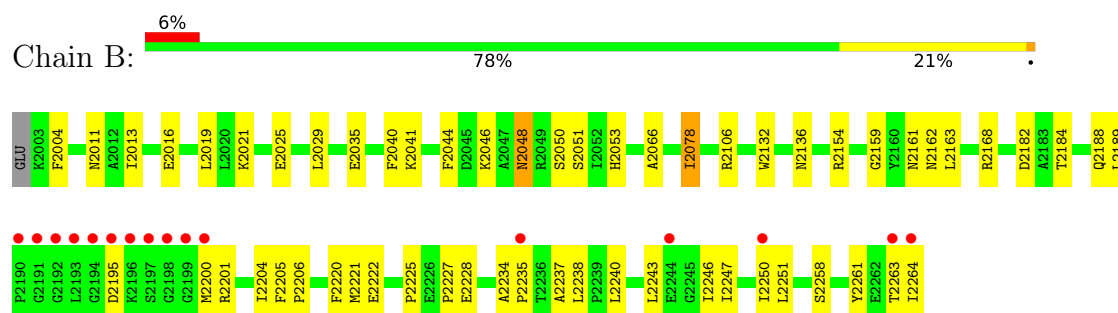
3 Residue-property plots [i](#)

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.

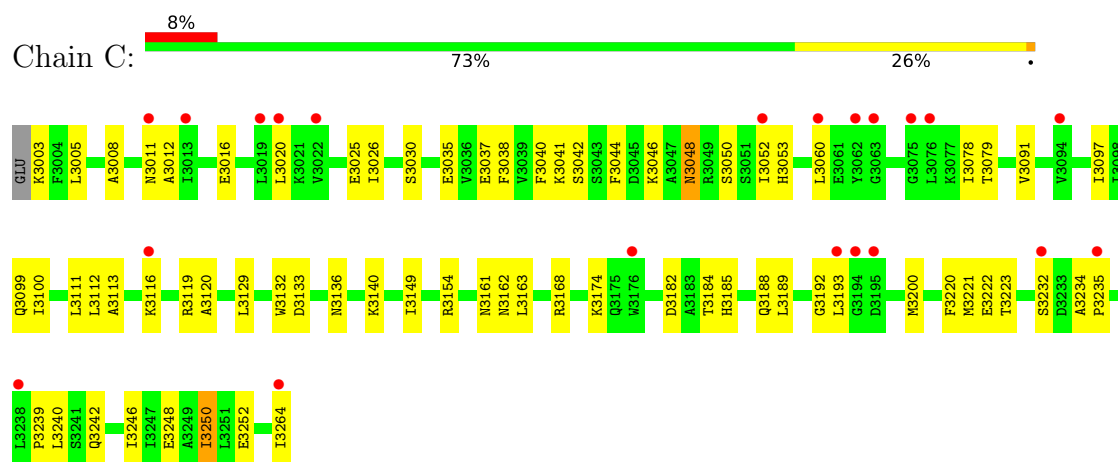
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



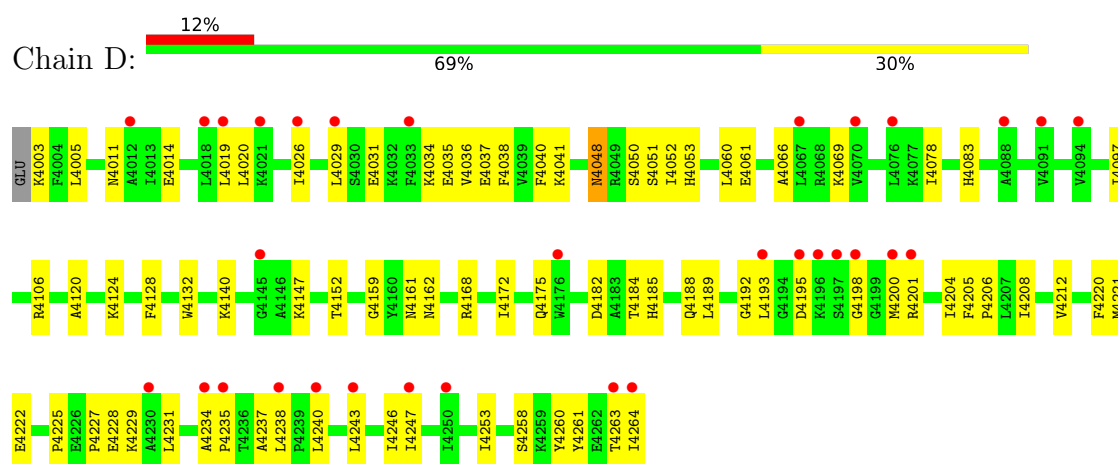
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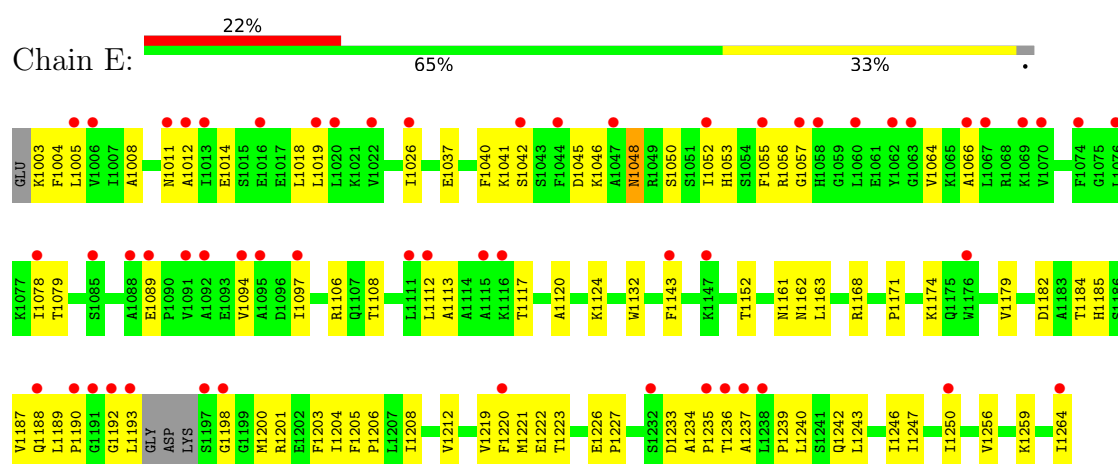
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



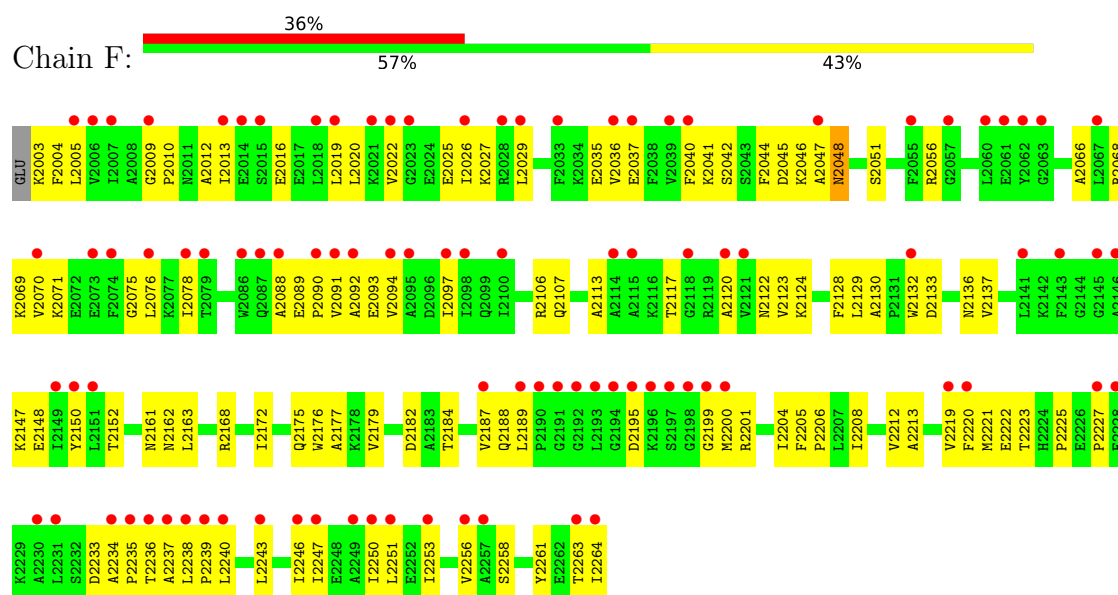
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



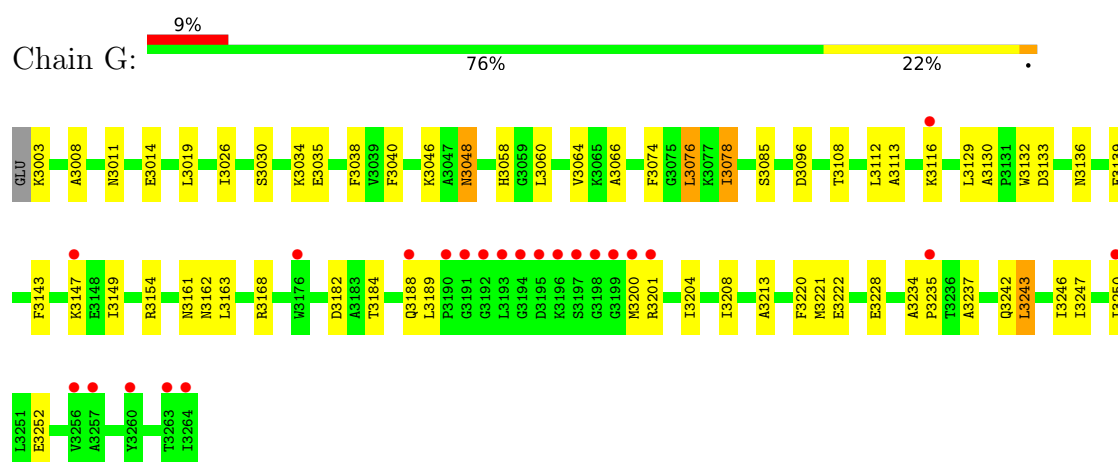
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



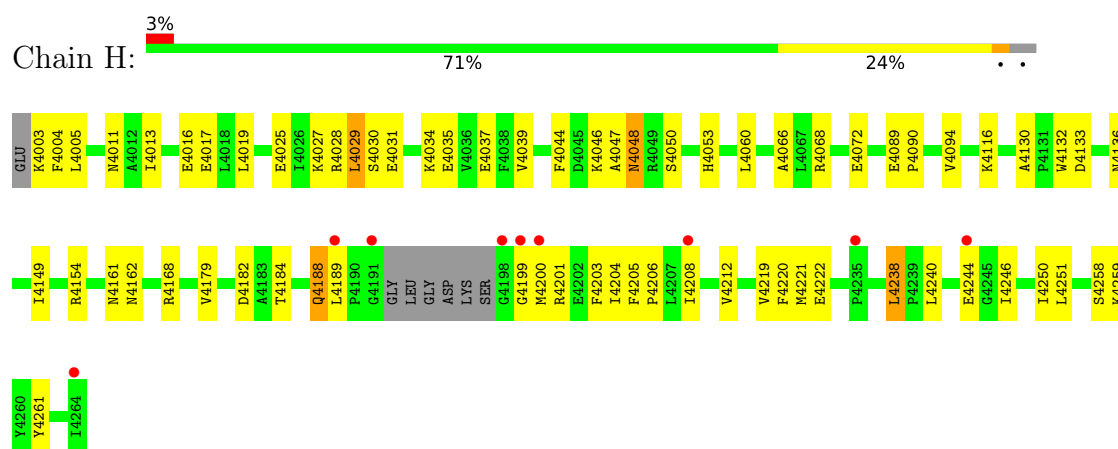
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



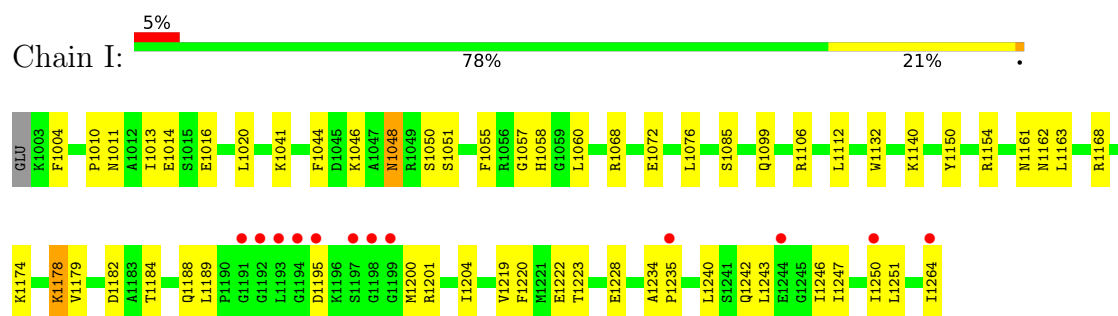
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



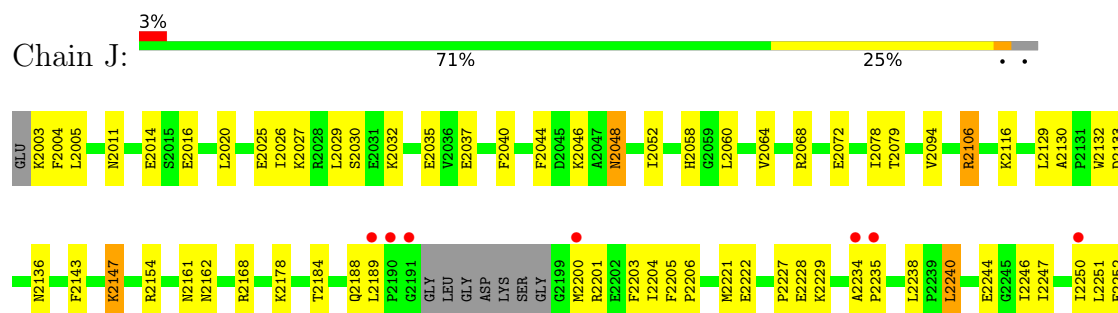
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



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

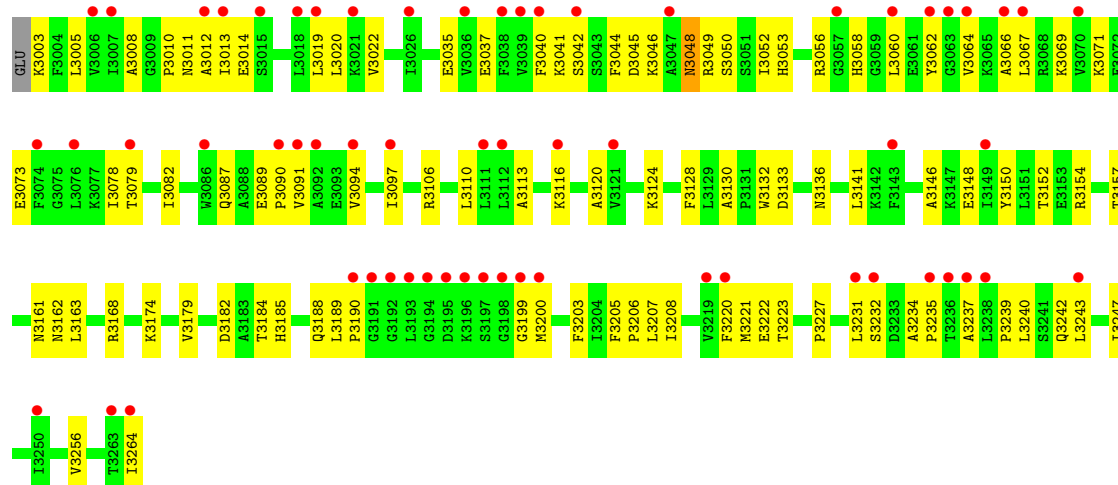


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

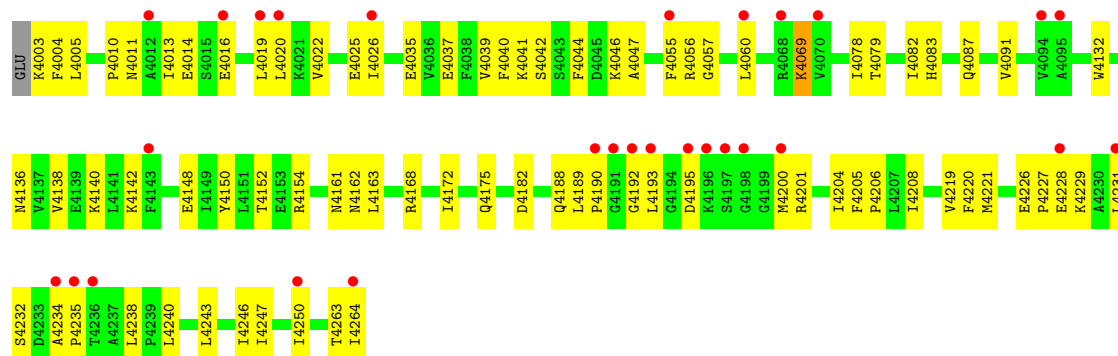




- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



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



4 Data and refinement statistics

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) 91.7 (30.18-2.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.245 0.205 , 0.245	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)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, 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	0.43	0/2098	0.87	1/2830 (0.0%)
1	B	0.43	0/2098	0.87	1/2830 (0.0%)
1	C	0.36	0/2098	0.81	1/2830 (0.0%)
1	D	0.34	0/2098	0.81	0/2830
1	E	0.33	0/2076	0.80	1/2800 (0.0%)
1	F	0.31	0/2098	0.78	1/2830 (0.0%)
1	G	0.40	0/2098	0.88	6/2830 (0.2%)
1	H	0.42	0/2058	0.85	2/2776 (0.1%)
1	I	0.43	0/2098	0.89	3/2830 (0.1%)
1	J	0.40	0/2054	0.86	0/2771
1	K	0.33	0/2098	0.79	1/2830 (0.0%)
1	L	0.34	0/2098	0.82	3/2830 (0.1%)
All	All	0.38	0/25070	0.84	20/33817 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3085	SER	N-CA-C	6.73	119.47	111.33
1	H	4179	VAL	N-CA-C	5.80	116.29	108.17
1	A	1179	VAL	N-CA-C	5.67	116.05	108.11
1	K	3179	VAL	N-CA-C	5.67	116.11	108.17
1	I	1178	LYS	N-CA-C	-5.52	102.72	110.50
1	G	3078	ILE	N-CA-C	5.47	116.36	108.48
1	C	3149	ILE	N-CA-C	5.36	115.68	108.17
1	I	1179	VAL	N-CA-C	5.33	115.57	108.11
1	G	3129	LEU	N-CA-C	5.32	118.49	109.76
1	L	4152	THR	N-CA-C	5.31	117.18	108.52
1	F	2179	VAL	N-CA-C	5.31	115.60	108.17
1	I	1085	SER	N-CA-C	5.28	117.44	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3096	ASP	N-CA-C	-5.16	106.14	112.90
1	L	4226	GLU	CA-C-N	5.12	125.16	119.32
1	L	4226	GLU	C-N-CA	5.12	125.16	119.32
1	G	3149	ILE	N-CA-C	5.10	116.06	108.46
1	E	1179	VAL	N-CA-C	5.09	115.29	108.17
1	B	2078	ILE	N-CA-C	5.06	116.64	108.85
1	G	3108	THR	N-CA-C	5.05	117.17	111.11
1	H	4149	ILE	N-CA-C	5.03	115.15	108.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2056	0	2095	52	0
1	B	2056	0	2095	56	0
1	C	2056	0	2095	64	0
1	D	2056	0	2095	64	0
1	E	2035	0	2074	65	0
1	F	2056	0	2095	85	0
1	G	2056	0	2095	50	0
1	H	2017	0	2055	65	0
1	I	2056	0	2095	54	0
1	J	2013	0	2052	72	0
1	K	2056	0	2095	72	0
1	L	2056	0	2095	67	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
4	B	190	0	0	3	0
4	C	107	0	0	2	0
4	D	75	0	0	4	0
4	E	64	0	0	5	0
4	F	54	0	0	5	0
4	G	178	0	0	3	0
4	H	170	0	0	7	0
4	I	185	0	0	4	0
4	J	172	0	0	7	0
4	K	50	0	0	4	0
4	L	99	0	0	5	0
All	All	26278	0	25060	709	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 (709) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2189:LEU:HD11	1:B:2200:MET:HE2	1.53	0.89
1:F:2189:LEU:HD21	1:F:2200:MET:HE2	1.52	0.89
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:E:1189:LEU:HD21	1:E:1200:MET:HE2	1.57	0.86
1:H:4189:LEU:HD21	1:H:4200:MET:HE2	1.58	0.86
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:C:3189:LEU:HD21	1:C:3200:MET:HE2	1.62	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:K:3189:LEU:HD21	1:K:3200:MET:HE2	1.63	0.80
1:C:3132:TRP:HE1	1:D:4161:ASN:HD21	1.28	0.80
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:H:4221:MET:HE3	1:H:4238:LEU:HD23	1.65	0.77
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:L:4189:LEU:HD11	1:L:4200:MET:HE2	1.66	0.75
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:J:2221:MET:HE2	1:J:2238:LEU:CD2	2.18	0.73
1:A:1202:GLU:HG3	4:A:5449:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1189:LEU:HD11	1:A:1200:MET:HE2	1.75	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
4:B:6608:HOH:O	1:C:3200:MET:HE3	1.92	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
1:B:2221:MET:HE3	1:B:2238:LEU:CD1	2.25	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:4221:MET:HE3	1:H:4238:LEU:CD2	2.30	0.61
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:B:2189:LEU:HD21	1:B:2200:MET:HE3	1.81	0.61
1:F:2221:MET:HE3	1:F:2238:LEU:HD23	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:D:4200:MET:HE3	4:D:6030:HOH:O	1.99	0.61
1:E:1162:ASN:HD21	1:H:4168:ARG:HH12	1.49	0.61
1:F:2027:LYS:HA	1:F:2076:LEU:HD21	1.82	0.61
1:G:3189:LEU:HD11	1:G:3200:MET:HE2	1.83	0.61
1:F:2129:LEU:HG	1:F:2133:ASP:HB2	1.83	0.61
1:H:4025:GLU:HG2	1:H:4240:LEU:HD22	1.83	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:F:2200:MET:HE3	4:F:5965:HOH:O	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:4221:MET:HE3	1:L:4238:LEU:HD12	1.83	0.59
1:K:3005:LEU:HD12	1:K:3037:GLU:O	2.02	0.59
1:J:2189:LEU:HD21	1:J:2200:MET:HE2	1.83	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:F:2189:LEU:HD21	1:F:2200:MET:CE	2.31	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:L:4041:LYS:HD3	1:L:4041:LYS:C	2.29	0.58
1:C:3041:LYS:HD3	1:C:3041:LYS:C	2.29	0.58
1:H:4130:ALA:HB3	1:H:4133:ASP:OD2	2.04	0.58
1:L:4200:MET:HE3	4:L:5974:HOH:O	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
1:K:3052:ILE:HB	1:L:4140:LYS:HG2	1.85	0.58
1:D:4189:LEU:HD11	1:D:4200:MET:HE2	1.85	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4189:LEU:HD21	1:D:4200:MET:HE2	1.86	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:F:2091:VAL:C	1:F:2093:GLU:H	2.12	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:I:1189:LEU:HD21	1:I:1200:MET:HE2	1.85	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:J:2221:MET:HE1	1:J:2246:ILE:HG21	1.87	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:I:1189:LEU:HD11	1:I:1200:MET:HE2	1.87	0.56
1:J:2200:MET:HE3	4:K:6142:HOH:O	2.05	0.56
1:F:2026:ILE:HD12	1:F:2040:PHE:CD1	2.40	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:H:4028:ARG:HH22	1:H:4244:GLU:CD	2.13	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
1:E:1011:ASN:HD21	1:E:1046:LYS:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:K:3041:LYS:HD3	1:K:3041:LYS:C	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1189:LEU:HD21	1:A:1200:MET:HE2	1.91	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
4:F:6186:HOH:O	1:G:3200:MET:HE3	2.10	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:G:3161:ASN:HD21	1:H:4132:TRP:NE1	2.06	0.51
1:K:3003:LYS:HG3	1:K:3035:GLU:O	2.10	0.51
1:E:1161:ASN:HD21	1:F:2132:TRP:NE1	2.05	0.51
1:F:2041:LYS:C	1:F:2041:LYS:HD3	2.35	0.51
1:K:3243:LEU:O	1:K:3247:ILE:HG13	2.10	0.51
1:I:1168:ARG:HH12	1:L:4162:ASN:HD21	1.59	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:J:2147:LYS:HZ2	1:J:2147:LYS:HB3	1.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4016:GLU:O	1:L:4020:LEU:HG	2.12	0.50
1:A:1200:MET:HE3	4:D:5790:HOH:O	2.12	0.50
1:H:4068:ARG:O	1:H:4072:GLU:HG3	2.12	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:E:1192:GLY:C	1:E:1193:LEU:HD12	2.36	0.50
1:G:3130:ALA:HB3	1:G:3133:ASP:OD2	2.12	0.50
1:L:4221:MET:HE3	1:L:4238:LEU:CD1	2.42	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:I:1200:MET:HE3	4:L:5522:HOH:O	2.13	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:J:2221:MET:HE2	1:J:2238:LEU:HD23	1.93	0.49
1:H:4005:LEU:HD11	1:H:4039:VAL:HG23	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3136:ASN:HB3	1:D:4050:SER:O	2.13	0.49
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: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:C:3192:GLY:C	1:C:3193:LEU:HD12	2.38	0.48
1:E:1187:VAL:HG21	1:E:1204:ILE:HG12	1.95	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:L:4220:PHE:CD1	1:L:4220:PHE:C	2.91	0.48
1:B:2025:GLU:HG2	1:B:2240:LEU:HD22	1.95	0.48
1:B:2041:LYS:HD3	1:B:2041:LYS:C	2.38	0.48
1:D:4221:MET:HE3	1:D:4238:LEU:HD22	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1132:TRP:NE1	1:B:2161:ASN:HD21	2.05	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
4:J:6049:HOH:O	1:K:3200:MET:HE3	2.13	0.47
1:L:4044:PHE:CZ	1:L:4060:LEU:HD13	2.50	0.47
1:D:4041:LYS:HD3	1:D:4041:LYS:C	2.40	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:H:4189:LEU:HD21	1:H:4200:MET:CE	2.37	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: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:I:1041:LYS:HD3	1:I:1041:LYS:C	2.39	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
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: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: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:K:3078:ILE:HG22	1:K:3079:THR:N	2.30	0.46
1:K:3189:LEU:HD21	1:K:3200:MET:CE	2.39	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:F:2048:ASN:C	1:F:2048:ASN:ND2	2.73	0.46
1:F:2048:ASN:C	1:F:2048:ASN:HD22	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4089:GLU:HB3	1:H:4090:PRO:CD	2.46	0.46
1:E:1041:LYS:HD3	1:E:1041:LYS:C	2.41	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
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:B:2221:MET:HE3	1:B:2238:LEU:HD12	1.98	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:D:4192:GLY:C	1:D:4193:LEU:HD22	2.41	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:K:3048:ASN:C	1:K:3048:ASN:HD22	2.24	0.45
1:L:4082:ILE:HG22	1:L:4091:VAL:HG21	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1182:ASP:HA	1:A:1220:PHE:HB3	1.99	0.44
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:L:4227:PRO:C	1:L:4229:LYS:H	2.26	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: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: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:4060:LEU:HD23	1:D:4060:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:3184:THR:CG2	1:G:3222:GLU:H	2.28	0.43
1:G:3189:LEU:HD21	1:G:3200:MET:HE2	1.99	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:A:1077:LYS:NZ	4:A:6682:HOH:O	2.51	0.43
1:C:3161:ASN:HD21	1:D:4132:TRP:NE1	2.04	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:K:3048:ASN:C	1:K:3048:ASN:ND2	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:4203:PHE:C	1:H:4206:PRO:HD2	2.44	0.42
1:K:3069:LYS:HE3	1:K:3073:GLU:OE1	2.19	0.42
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:F:2220:PHE:CD1	1:F:2220:PHE:C	2.97	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:A:1252:GLU:OE1	1:D:4260:TYR:OH	2.33	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: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:D:4220:PHE:CD1	1:D:4220:PHE:C	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3124:LYS:HD3	1:K:3152:THR:HB	2.00	0.42
1:L:4192:GLY:C	1:L:4193:LEU:HD22	2.45	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: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
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: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:D:4011:ASN:HD22	1:D:4222:GLU:CD	2.29	0.41
1:I:1055:PHE:CZ	1:I:1057:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4221:MET:HE2	1:D:4243:LEU:CD1	2.51	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
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: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: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:I:1250:ILE:HG13	1:I:1251:LEU:N	2.36	0.40
1:J:2203:PHE:C	1:J:2206:PRO:HD2	2.46	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:J:2032:LYS:HE2	1:J:2244:GLU:CD	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	30	28
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%)	30	28
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%)	48	49

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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%)	212 (97%)	6 (3%)	38	42
1	B	218/219 (100%)	212 (97%)	6 (3%)	38	42
1	C	218/219 (100%)	215 (99%)	3 (1%)	59	67
1	D	218/219 (100%)	216 (99%)	2 (1%)	70	78
1	E	216/219 (99%)	213 (99%)	3 (1%)	59	67
1	F	218/219 (100%)	216 (99%)	2 (1%)	70	78
1	G	218/219 (100%)	213 (98%)	5 (2%)	44	50
1	H	214/219 (98%)	210 (98%)	4 (2%)	50	57
1	I	218/219 (100%)	215 (99%)	3 (1%)	59	67
1	J	214/219 (98%)	210 (98%)	4 (2%)	50	57
1	K	218/219 (100%)	217 (100%)	1 (0%)	81	87
1	L	218/219 (100%)	216 (99%)	2 (1%)	70	78
All	All	2606/2628 (99%)	2565 (98%)	41 (2%)	55	63

All (41) 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	1184	THR
1	A	1228	GLU
1	A	1243	LEU
1	B	2016	GLU
1	B	2029	LEU
1	B	2035	GLU

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Mol	Chain	Res	Type
1	B	2048	ASN
1	B	2106	ARG
1	B	2228	GLU
1	C	3048	ASN
1	C	3112	LEU
1	C	3250	ILE
1	D	4029	LEU
1	D	4048	ASN
1	E	1048	ASN
1	E	1089	GLU
1	E	1226	GLU
1	F	2016	GLU
1	F	2048	ASN
1	G	3048	ASN
1	G	3076	LEU
1	G	3112	LEU
1	G	3228	GLU
1	G	3243	LEU
1	H	4029	LEU
1	H	4048	ASN
1	H	4188	GLN
1	H	4238	LEU
1	I	1048	ASN
1	I	1076	LEU
1	I	1112	LEU
1	J	2048	ASN
1	J	2106	ARG
1	J	2147	LYS
1	J	2240	LEU
1	K	3048	ASN
1	L	4069	LYS
1	L	4243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) 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	1122	ASN
1	A	1136	ASN

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Mol	Chain	Res	Type
1	A	1161	ASN
1	A	1162	ASN
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	2099	GLN
1	B	2136	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	3175	GLN
1	C	3188	GLN
1	C	3242	GLN
1	D	4048	ASN
1	D	4058	HIS
1	D	4083	HIS
1	D	4099	GLN
1	D	4107	GLN
1	D	4122	ASN
1	D	4136	ASN
1	D	4161	ASN
1	D	4162	ASN
1	D	4185	HIS
1	D	4188	GLN
1	E	1011	ASN
1	E	1048	ASN
1	E	1053	HIS
1	E	1083	HIS
1	E	1136	ASN
1	E	1161	ASN
1	E	1162	ASN
1	E	1188	GLN

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Mol	Chain	Res	Type
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	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	3175	GLN
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
1	I	1058	HIS
1	I	1099	GLN
1	I	1161	ASN
1	I	1162	ASN
1	I	1175	GLN
1	I	1188	GLN
1	J	2011	ASN
1	J	2048	ASN
1	J	2058	HIS
1	J	2099	GLN
1	J	2122	ASN
1	J	2161	ASN
1	J	2162	ASN

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Mol	Chain	Res	Type
1	J	2188	GLN
1	J	2242	GLN
1	K	3048	ASN
1	K	3053	HIS
1	K	3099	GLN
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	4083	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 oligosaccharides 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	K	1290	-	4,4,4	1.74	1 (25%)	6,6,6	0.48	0
2	PO4	B	1281	-	4,4,4	1.68	0	6,6,6	0.47	0
3	PEP	K	1278	-	9,9,9	1.09	0	11,13,13	1.41	2 (18%)
3	PEP	A	1268	-	9,9,9	0.83	0	11,13,13	1.59	1 (9%)
3	PEP	B	1269	-	9,9,9	1.00	0	11,13,13	1.59	2 (18%)
2	PO4	J	1289	-	4,4,4	1.72	1 (25%)	6,6,6	0.45	0
2	PO4	F	1285	-	4,4,4	1.70	0	6,6,6	0.47	0
3	PEP	H	1275	-	9,9,9	0.91	0	11,13,13	1.27	2 (18%)
3	PEP	C	1270	-	9,9,9	1.12	0	11,13,13	1.66	2 (18%)
3	PEP	J	1277	-	9,9,9	0.80	0	11,13,13	1.48	3 (27%)
2	PO4	L	1291	-	4,4,4	1.68	0	6,6,6	0.48	0
3	PEP	I	1276	-	9,9,9	0.82	0	11,13,13	1.29	1 (9%)
2	PO4	E	1284	-	4,4,4	1.69	0	6,6,6	0.47	0
3	PEP	F	1273	-	9,9,9	1.10	0	11,13,13	1.53	2 (18%)
3	PEP	D	1271	-	9,9,9	0.94	0	11,13,13	1.71	2 (18%)
3	PEP	G	1274	-	9,9,9	1.02	0	11,13,13	1.61	1 (9%)
2	PO4	H	1287	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PEP	L	1279	-	9,9,9	1.04	0	11,13,13	1.50	2 (18%)
2	PO4	D	1283	-	4,4,4	1.71	0	6,6,6	0.49	0
2	PO4	A	1280	-	4,4,4	1.66	1 (25%)	6,6,6	0.46	0
2	PO4	G	1286	-	4,4,4	1.64	0	6,6,6	0.48	0
2	PO4	I	1288	-	4,4,4	1.67	0	6,6,6	0.47	0
3	PEP	E	1272	-	9,9,9	1.06	0	11,13,13	1.70	3 (27%)
2	PO4	C	1282	-	4,4,4	1.70	0	6,6,6	0.48	0

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	K	1278	-	-	4/9/9/9	-
3	PEP	F	1273	-	-	0/9/9/9	-
3	PEP	A	1268	-	-	0/9/9/9	-
3	PEP	D	1271	-	-	0/9/9/9	-
3	PEP	H	1275	-	-	0/9/9/9	-
3	PEP	G	1274	-	-	0/9/9/9	-
3	PEP	C	1270	-	-	0/9/9/9	-
3	PEP	B	1269	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEP	E	1272	-	-	1/9/9/9	-
3	PEP	J	1277	-	-	0/9/9/9	-
3	PEP	L	1279	-	-	0/9/9/9	-
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)
2	A	1280	PO4	P-O3	-2.08	1.48	1.54
2	J	1289	PO4	P-O3	-2.07	1.48	1.54
2	K	1290	PO4	P-O3	-2.02	1.48	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	-2.93	116.92	123.90
3	F	1273	PEP	O2'-C1-O1	-2.88	117.03	123.90
3	L	1279	PEP	O2'-C1-O1	-2.62	117.65	123.90
3	D	1271	PEP	O2'-C1-O1	-2.60	117.71	123.90
3	K	1278	PEP	O2'-C1-O1	-2.58	117.75	123.90
3	C	1270	PEP	O2'-C1-O1	-2.51	117.93	123.90
3	J	1277	PEP	O3P-P-O1P	2.35	119.98	110.83
3	B	1269	PEP	O2'-C1-O1	-2.27	118.50	123.90
3	H	1275	PEP	O2'-C1-O1	-2.12	118.84	123.90
3	J	1277	PEP	O2'-C1-O1	-2.07	118.98	123.90
3	E	1272	PEP	O2-C2-C3	-2.04	120.95	124.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
3	E	1272	PEP	C2-O2-P-O1P

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 ⓘ

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, 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%)	-0.07	13 (4%) 34 37	15, 24, 46, 69	0
1	B	262/263 (99%)	0.00	16 (6%) 27 29	13, 24, 47, 78	0
1	C	262/263 (99%)	0.62	21 (8%) 18 20	19, 41, 57, 67	0
1	D	262/263 (99%)	0.99	32 (12%) 8 9	21, 44, 65, 79	0
1	E	259/263 (98%)	1.19	57 (22%) 2 2	23, 52, 71, 79	0
1	F	262/263 (99%)	1.72	95 (36%) 1 1	25, 57, 75, 83	0
1	G	262/263 (99%)	0.22	23 (8%) 15 17	17, 29, 59, 77	0
1	H	256/263 (97%)	0.00	9 (3%) 47 50	15, 26, 47, 79	0
1	I	262/263 (99%)	-0.04	12 (4%) 37 40	15, 25, 47, 73	0
1	J	255/263 (96%)	-0.07	8 (3%) 51 54	14, 27, 49, 75	0
1	K	262/263 (99%)	1.37	61 (23%) 2 2	26, 56, 73, 77	0
1	L	262/263 (99%)	0.86	28 (10%) 11 12	22, 45, 62, 79	0
All	All	3128/3156 (99%)	0.57	375 (11%) 9 9	13, 36, 68, 83	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2197	SER	6.6
1	I	1198	GLY	5.8
1	H	4264	ILE	5.8
1	E	1191	GLY	5.6
1	F	2264	ILE	5.4
1	F	2193	LEU	5.3
1	D	4264	ILE	5.2
1	A	1195	ASP	5.2
1	J	2264	ILE	5.1
1	B	2195	ASP	5.1
1	I	1197	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	2198	GLY	5.0
1	L	4198	GLY	4.9
1	L	4264	ILE	4.9
1	D	4197	SER	4.9
1	A	1193	LEU	4.7
1	K	3197	SER	4.7
1	D	4198	GLY	4.7
1	I	1193	LEU	4.6
1	F	2250	ILE	4.6
1	K	3250	ILE	4.6
1	H	4235	PRO	4.5
1	F	2197	SER	4.5
1	K	3194	GLY	4.5
1	K	3264	ILE	4.5
1	G	3264	ILE	4.5
1	K	3076	LEU	4.5
1	B	2194	GLY	4.4
1	K	3060	LEU	4.4
1	F	2022	VAL	4.3
1	C	3193	LEU	4.3
1	D	4195	ASP	4.3
1	E	1091	VAL	4.3
1	E	1198	GLY	4.3
1	B	2196	LYS	4.3
1	L	4195	ASP	4.2
1	B	2193	LEU	4.2
1	B	2264	ILE	4.1
1	F	2198	GLY	4.1
1	E	1197	SER	4.1
1	K	3018	LEU	4.0
1	L	4060	LEU	4.0
1	G	3193	LEU	3.9
1	L	4193	LEU	3.9
1	F	2057	GLY	3.9
1	F	2249	ALA	3.9
1	C	3020	LEU	3.9
1	B	2199	GLY	3.9
1	J	2235	PRO	3.9
1	D	4193	LEU	3.9
1	F	2019	LEU	3.9
1	K	3198	GLY	3.8
1	K	3200	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	1199	GLY	3.8
1	K	3063	GLY	3.8
1	L	4235	PRO	3.7
1	D	4250	ILE	3.7
1	F	2150	TYR	3.7
1	E	1060	LEU	3.7
1	E	1264	ILE	3.7
1	K	3235	PRO	3.6
1	G	3196	LYS	3.6
1	A	1264	ILE	3.6
1	A	1198	GLY	3.6
1	F	2121	VAL	3.6
1	B	2191	GLY	3.6
1	G	3194	GLY	3.6
1	F	2005	LEU	3.6
1	G	3197	SER	3.6
1	E	1012	ALA	3.5
1	K	3019	LEU	3.5
1	L	4020	LEU	3.5
1	L	4196	LYS	3.5
1	F	2191	GLY	3.5
1	F	2097	ILE	3.5
1	B	2235	PRO	3.5
1	F	2141	LEU	3.5
1	F	2095	ALA	3.4
1	K	3195	ASP	3.4
1	E	1076	LEU	3.4
1	K	3193	LEU	3.4
1	C	3195	ASP	3.3
1	C	3264	ILE	3.3
1	F	2060	LEU	3.3
1	B	2192	GLY	3.3
1	A	1194	GLY	3.3
1	F	2194	GLY	3.3
1	I	1194	GLY	3.3
1	F	2007	ILE	3.3
1	F	2018	LEU	3.3
1	A	1191	GLY	3.2
1	H	4198	GLY	3.2
1	F	2062	TYR	3.2
1	F	2029	LEU	3.2
1	K	3196	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	3195	ASP	3.2
1	J	2191	GLY	3.2
1	F	2006	VAL	3.2
1	F	2094	VAL	3.2
1	J	2200	MET	3.2
1	F	2026	ILE	3.2
1	G	3199	GLY	3.2
1	H	4199	GLY	3.2
1	K	3057	GLY	3.2
1	F	2235	PRO	3.2
1	G	3250	ILE	3.2
1	F	2195	ASP	3.2
1	I	1264	ILE	3.1
1	F	2220	PHE	3.1
1	L	4192	GLY	3.1
1	G	3190	PRO	3.1
1	G	3198	GLY	3.1
1	D	4196	LYS	3.1
1	C	3060	LEU	3.1
1	D	4076	LEU	3.1
1	F	2196	LYS	3.0
1	L	4190	PRO	3.0
1	F	2074	PHE	3.0
1	F	2070	VAL	3.0
1	K	3091	VAL	3.0
1	K	3192	GLY	3.0
1	E	1237	ALA	3.0
1	F	2238	LEU	3.0
1	K	3006	VAL	3.0
1	F	2098	ILE	3.0
1	I	1192	GLY	3.0
1	G	3263	THR	3.0
1	K	3074	PHE	3.0
1	F	2246	ILE	2.9
1	H	4208	ILE	2.9
1	E	1116	LYS	2.9
1	K	3062	TYR	2.9
1	D	4234	ALA	2.9
1	E	1095	ALA	2.9
1	B	2190	PRO	2.9
1	E	1192	GLY	2.9
1	F	2023	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	3067	LEU	2.9
1	F	2013	ILE	2.9
1	A	1196	LYS	2.9
1	F	2143	PHE	2.9
1	E	1070	VAL	2.8
1	K	3097	ILE	2.8
1	A	1235	PRO	2.8
1	F	2227	PRO	2.8
1	G	3235	PRO	2.8
1	F	2033	PHE	2.8
1	F	2199	GLY	2.8
1	F	2230	ALA	2.8
1	F	2251	LEU	2.8
1	E	1022	VAL	2.8
1	B	2250	ILE	2.8
1	J	2250	ILE	2.8
1	K	3243	LEU	2.8
1	E	1094	VAL	2.8
1	K	3070	VAL	2.8
1	E	1052	ILE	2.8
1	E	1057	GLY	2.8
1	E	1074	PHE	2.8
1	K	3066	ALA	2.8
1	E	1111	LEU	2.8
1	D	4235	PRO	2.8
1	F	2100	ILE	2.8
1	I	1195	ASP	2.7
1	E	1063	GLY	2.7
1	E	1143	PHE	2.7
1	K	3231	LEU	2.7
1	F	2090	PRO	2.7
1	D	4247	ILE	2.7
1	F	2040	PHE	2.7
1	F	2146	ALA	2.7
1	E	1193	LEU	2.7
1	F	2263	THR	2.7
1	G	3260	TYR	2.7
1	K	3094	VAL	2.7
1	K	3219	VAL	2.7
1	L	4094	VAL	2.7
1	F	2149	ILE	2.7
1	A	1197	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1199	GLY	2.7
1	F	2055	PHE	2.7
1	F	2088	ALA	2.7
1	K	3047	ALA	2.7
1	K	3092	ALA	2.7
1	D	4018	LEU	2.7
1	I	1235	PRO	2.7
1	F	2039	VAL	2.7
1	G	3188	GLN	2.6
1	D	4012	ALA	2.6
1	E	1089	GLU	2.6
1	F	2120	ALA	2.6
1	I	1244	GLU	2.6
1	K	3012	ALA	2.6
1	F	2200	MET	2.6
1	D	4026	ILE	2.6
1	E	1250	ILE	2.6
1	F	2118	GLY	2.6
1	E	1092	ALA	2.6
1	A	1250	ILE	2.6
1	E	1013	ILE	2.6
1	K	3036	VAL	2.6
1	K	3191	GLY	2.6
1	K	3007	ILE	2.6
1	K	3079	THR	2.6
1	E	1026	ILE	2.5
1	E	1190	PRO	2.5
1	K	3232	SER	2.5
1	D	4019	LEU	2.5
1	K	3238	LEU	2.5
1	K	3038	PHE	2.5
1	D	4200	MET	2.5
1	F	2009	GLY	2.5
1	K	3090	PRO	2.5
1	E	1019	LEU	2.5
1	E	1112	LEU	2.5
1	E	1238	LEU	2.5
1	C	3063	GLY	2.5
1	C	3116	LYS	2.5
1	E	1097	ILE	2.5
1	F	2078	ILE	2.5
1	G	3256	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	2087	GLN	2.5
1	D	4240	LEU	2.5
1	D	4243	LEU	2.5
1	F	2189	LEU	2.5
1	K	3112	LEU	2.5
1	L	4143	PHE	2.5
1	F	2247	ILE	2.5
1	K	3026	ILE	2.5
1	K	3121	VAL	2.4
1	F	2092	ALA	2.4
1	C	3194	GLY	2.4
1	H	4191	GLY	2.4
1	F	2091	VAL	2.4
1	K	3013	ILE	2.4
1	J	2190	PRO	2.4
1	F	2237	ALA	2.4
1	K	3237	ALA	2.4
1	F	2076	LEU	2.4
1	F	2151	LEU	2.4
1	H	4189	LEU	2.4
1	C	3075	GLY	2.4
1	D	4094	VAL	2.4
1	L	4068	ARG	2.4
1	F	2047	ALA	2.4
1	J	2234	ALA	2.4
1	D	4238	LEU	2.4
1	F	2061	GLU	2.4
1	C	3094	VAL	2.4
1	E	1006	VAL	2.4
1	F	2236	THR	2.4
1	L	4228	GLU	2.3
1	L	4234	ALA	2.3
1	C	3011	ASN	2.3
1	C	3076	LEU	2.3
1	D	4029	LEU	2.3
1	E	1078	ILE	2.3
1	D	4070	VAL	2.3
1	F	2036	VAL	2.3
1	E	1236	THR	2.3
1	L	4236	THR	2.3
1	F	2234	ALA	2.3
1	F	2243	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	1147	LYS	2.3
1	C	3052	ILE	2.3
1	F	2228	GLU	2.3
1	K	3064	VAL	2.3
1	C	3235	PRO	2.3
1	D	4263	THR	2.3
1	E	1047	ALA	2.3
1	F	2114	ALA	2.3
1	A	1189	LEU	2.3
1	G	3176	TRP	2.3
1	L	4019	LEU	2.3
1	E	1220	PHE	2.3
1	H	4244	GLU	2.3
1	L	4016	GLU	2.3
1	C	3022	VAL	2.3
1	K	3190	PRO	2.3
1	K	3236	THR	2.3
1	L	4191	GLY	2.3
1	C	3019	LEU	2.3
1	G	3200	MET	2.3
1	F	2132	TRP	2.3
1	B	2244	GLU	2.2
1	E	1058	HIS	2.2
1	F	2037	GLU	2.2
1	F	2015	SER	2.2
1	K	3220	PHE	2.2
1	F	2253	ILE	2.2
1	I	1250	ILE	2.2
1	F	2256	VAL	2.2
1	D	4230	ALA	2.2
1	E	1088	ALA	2.2
1	G	3192	GLY	2.2
1	C	3238	LEU	2.2
1	E	1020	LEU	2.2
1	L	4231	LEU	2.2
1	E	1016	GLU	2.2
1	D	4033	PHE	2.2
1	B	2263	THR	2.2
1	F	2190	PRO	2.2
1	B	2200	MET	2.2
1	F	2257	ALA	2.2
1	C	3062	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	3015	SER	2.2
1	K	3042	SER	2.2
1	L	4197	SER	2.2
1	D	4176	TRP	2.2
1	G	3147	LYS	2.2
1	F	2079	THR	2.2
1	K	3040	PHE	2.2
1	L	4200	MET	2.2
1	F	2187	VAL	2.2
1	K	3199	GLY	2.2
1	E	1115	ALA	2.2
1	L	4012	ALA	2.2
1	E	1005	LEU	2.2
1	E	1232	SER	2.2
1	K	3116	LYS	2.2
1	K	3143	PHE	2.1
1	L	4055	PHE	2.1
1	L	4250	ILE	2.1
1	D	4091	VAL	2.1
1	L	4070	VAL	2.1
1	F	2115	ALA	2.1
1	L	4095	ALA	2.1
1	D	4067	LEU	2.1
1	E	1067	LEU	2.1
1	F	2067	LEU	2.1
1	D	4021	LYS	2.1
1	F	2021	LYS	2.1
1	F	2014	GLU	2.1
1	C	3013	ILE	2.1
1	E	1066	ALA	2.1
1	F	2231	LEU	2.1
1	F	2240	LEU	2.1
1	G	3116	LYS	2.1
1	C	3232	SER	2.1
1	E	1062	TYR	2.1
1	E	1235	PRO	2.1
1	F	2028	ARG	2.1
1	F	2145	GLY	2.1
1	G	3191	GLY	2.1
1	L	4026	ILE	2.1
1	C	3176	TRP	2.1
1	D	4088	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1085	SER	2.1
1	J	2189	LEU	2.1
1	H	4200	MET	2.1
1	E	1011	ASN	2.1
1	G	3201	ARG	2.1
1	D	4145	GLY	2.1
1	F	2063	GLY	2.1
1	I	1191	GLY	2.1
1	E	1069	LYS	2.1
1	E	1044	PHE	2.1
1	E	1055	PHE	2.1
1	F	2219	VAL	2.1
1	K	3039	VAL	2.1
1	F	2086	TRP	2.1
1	E	1042	SER	2.1
1	G	3257	ALA	2.1
1	K	3111	LEU	2.0
1	E	1188	GLN	2.0
1	K	3263	THR	2.0
1	K	3021	LYS	2.0
1	K	3149	ILE	2.0
1	A	1228	GLU	2.0
1	F	2073	GLU	2.0
1	E	1176	TRP	2.0
1	K	3086	TRP	2.0
1	D	4201	ARG	2.0
1	F	2239	PRO	2.0
1	F	2192	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	D	1283	5/5	0.86	0.12	57,58,60,61	0
2	PO4	E	1284	5/5	0.86	0.10	70,70,71,71	0
2	PO4	K	1290	5/5	0.88	0.11	61,61,62,62	0
2	PO4	L	1291	5/5	0.89	0.12	60,60,61,61	0
2	PO4	F	1285	5/5	0.90	0.10	62,63,64,64	0
2	PO4	C	1282	5/5	0.92	0.09	47,50,51,51	0
3	PEP	F	1273	10/10	0.93	0.10	40,46,48,48	0
2	PO4	H	1287	5/5	0.94	0.08	37,39,40,41	0
3	PEP	E	1272	10/10	0.94	0.09	42,46,50,50	0
2	PO4	B	1281	5/5	0.94	0.08	32,36,38,38	0
3	PEP	K	1278	10/10	0.94	0.10	40,45,49,50	0
2	PO4	I	1288	5/5	0.95	0.07	33,35,37,38	0
2	PO4	G	1286	5/5	0.95	0.10	35,37,39,39	0
3	PEP	D	1271	10/10	0.96	0.08	29,35,40,42	0
2	PO4	J	1289	5/5	0.96	0.07	38,40,42,43	0
3	PEP	L	1279	10/10	0.96	0.07	32,37,41,43	0
3	PEP	C	1270	10/10	0.97	0.07	28,35,37,39	0
2	PO4	A	1280	5/5	0.97	0.06	31,33,35,37	0
3	PEP	G	1274	10/10	0.98	0.05	18,23,25,26	0
3	PEP	H	1275	10/10	0.99	0.03	15,21,23,24	0
3	PEP	I	1276	10/10	0.99	0.05	17,21,22,23	0
3	PEP	J	1277	10/10	0.99	0.04	16,20,22,22	0
3	PEP	B	1269	10/10	0.99	0.04	14,17,22,26	0
3	PEP	A	1268	10/10	0.99	0.04	15,19,23,23	0

6.5 Other polymers

There are no such residues in this entry.