



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 AM GMT

PDB ID : 2NX3
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 : 2006-11-16
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

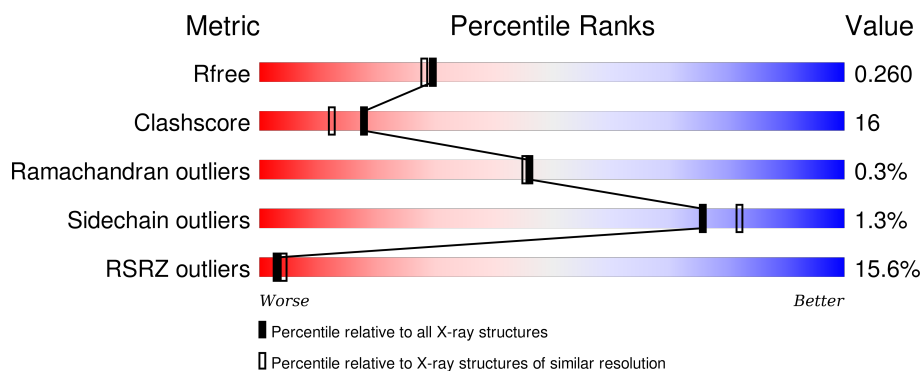
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	<div> <div>4%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	267	<div> <div>7%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	C	267	<div> <div>12%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	D	267	<div> <div>22%</div> <div>64%</div> <div>33%</div> <div>..</div> </div>
1	E	267	<div> <div>27%</div> <div>63%</div> <div>33%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	267	
1	G	267	
1	H	267	
1	I	267	
1	J	267	
1	K	267	
1	L	267	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEP	B	268	-	-	X	-
2	PEP	H	268	-	-	X	-
2	PEP	I	268	-	-	X	-
3	A5P	B	269	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26573 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
			2055	1327	344	379	5			
1	B	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	C	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	D	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	E	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	F	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	G	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	H	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	I	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	J	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	K	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			
1	L	262	Total	C	N	O	S	0	0	0
			2055	1327	344	379	5			

There are 36 discrepancies between the modelled and reference sequences:

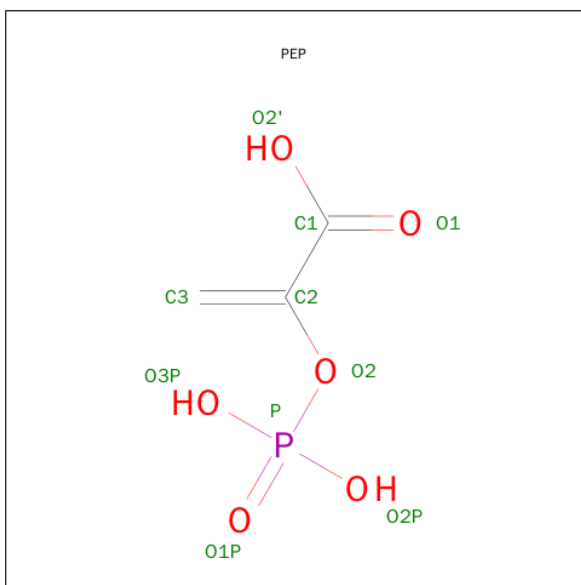
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ASN	CYS	ENGINEERED	UNP O66496
A	235	PRO	SER	ENGINEERED	UNP O66496
A	237	ALA	GLN	ENGINEERED	UNP O66496
B	11	ASN	CYS	ENGINEERED	UNP O66496
B	235	PRO	SER	ENGINEERED	UNP O66496

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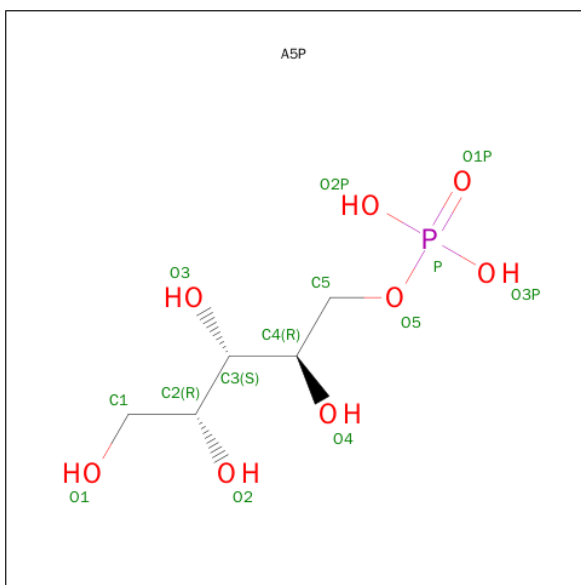
Chain	Residue	Modelled	Actual	Comment	Reference
B	237	ALA	GLN	ENGINEERED	UNP O66496
C	11	ASN	CYS	ENGINEERED	UNP O66496
C	235	PRO	SER	ENGINEERED	UNP O66496
C	237	ALA	GLN	ENGINEERED	UNP O66496
D	11	ASN	CYS	ENGINEERED	UNP O66496
D	235	PRO	SER	ENGINEERED	UNP O66496
D	237	ALA	GLN	ENGINEERED	UNP O66496
E	11	ASN	CYS	ENGINEERED	UNP O66496
E	235	PRO	SER	ENGINEERED	UNP O66496
E	237	ALA	GLN	ENGINEERED	UNP O66496
F	11	ASN	CYS	ENGINEERED	UNP O66496
F	235	PRO	SER	ENGINEERED	UNP O66496
F	237	ALA	GLN	ENGINEERED	UNP O66496
G	11	ASN	CYS	ENGINEERED	UNP O66496
G	235	PRO	SER	ENGINEERED	UNP O66496
G	237	ALA	GLN	ENGINEERED	UNP O66496
H	11	ASN	CYS	ENGINEERED	UNP O66496
H	235	PRO	SER	ENGINEERED	UNP O66496
H	237	ALA	GLN	ENGINEERED	UNP O66496
I	11	ASN	CYS	ENGINEERED	UNP O66496
I	235	PRO	SER	ENGINEERED	UNP O66496
I	237	ALA	GLN	ENGINEERED	UNP O66496
J	11	ASN	CYS	ENGINEERED	UNP O66496
J	235	PRO	SER	ENGINEERED	UNP O66496
J	237	ALA	GLN	ENGINEERED	UNP O66496
K	11	ASN	CYS	ENGINEERED	UNP O66496
K	235	PRO	SER	ENGINEERED	UNP O66496
K	237	ALA	GLN	ENGINEERED	UNP O66496
L	11	ASN	CYS	ENGINEERED	UNP O66496
L	235	PRO	SER	ENGINEERED	UNP O66496
L	237	ALA	GLN	ENGINEERED	UNP O66496

- Molecule 2 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C₃H₅O₆P).



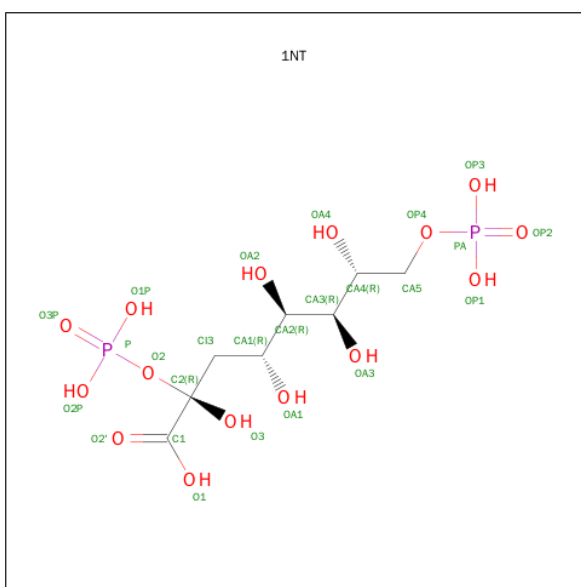
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	F	1	Total	C	O	P	0	0
			10	3	6	1		
2	G	1	Total	C	O	P	0	0
			10	3	6	1		
2	H	1	Total	C	O	P	0	0
			10	3	6	1		
2	I	1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

- Molecule 3 is ARABINOSE-5-PHOSPHATE (three-letter code: A5P) (formula: C₅H₁₃O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	8	1		
3	B	1	Total	C	O	P	0	0
			14	5	8	1		
3	C	1	Total	C	O	P	0	0
			14	5	8	1		
3	E	1	Total	C	O	P	0	0
			14	5	8	1		
3	F	1	Total	C	O	P	0	0
			14	5	8	1		
3	G	1	Total	C	O	P	0	0
			14	5	8	1		
3	H	1	Total	C	O	P	0	0
			14	5	8	1		
3	I	1	Total	C	O	P	0	0
			14	5	8	1		
3	J	1	Total	C	O	P	0	0
			14	5	8	1		
3	K	1	Total	C	O	P	0	0
			14	5	8	1		
3	L	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 4 is (2R,4R,5R,6R,7R)-2,4,5,6,7-PENTAHYDROXY-2,8-BIS(PHOSPHONOOXY)OCTANOIC ACID (three-letter code: 1NT) (formula: C₈H₁₈O₁₅P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	P	0	0
			25	8	15	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	194	Total O 194 194	0	0
5	B	197	Total O 197 197	0	0
5	C	108	Total O 108 108	0	0
5	D	88	Total O 88 88	0	0
5	E	71	Total O 71 71	0	0
5	F	55	Total O 55 55	0	0
5	G	177	Total O 177 177	0	0
5	H	191	Total O 191 191	0	0
5	I	191	Total O 191 191	0	0
5	J	184	Total O 184 184	0	0
5	K	56	Total O 56 56	0	0

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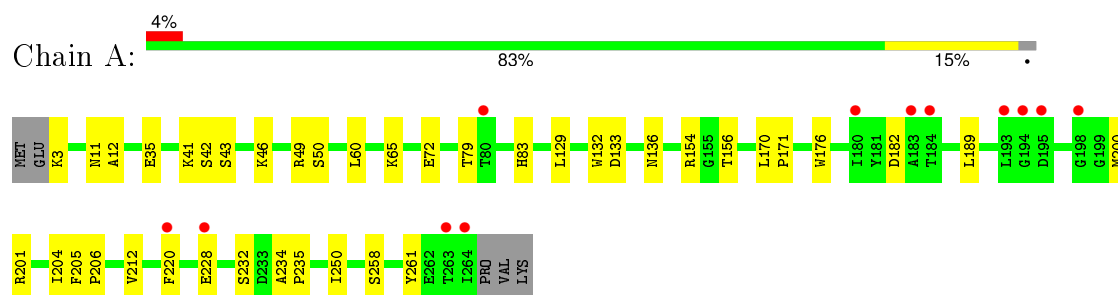
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	112	Total	O	0	0
			112	112		

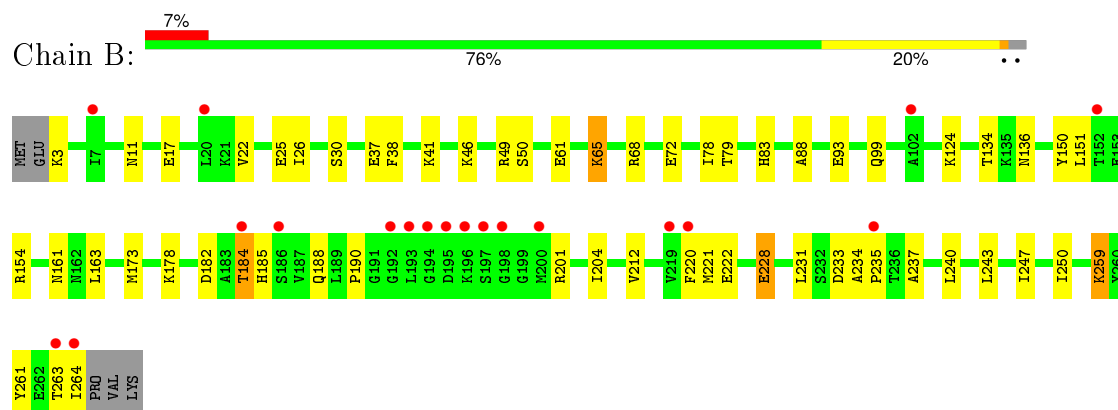
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

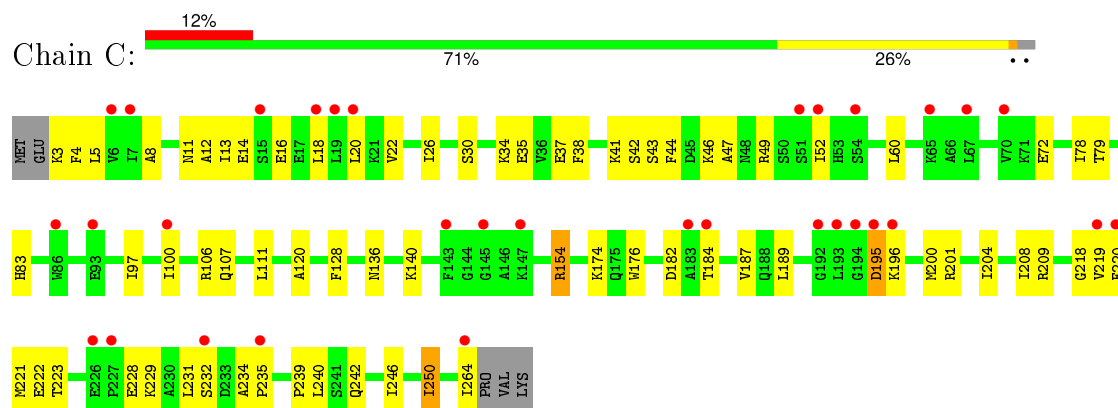
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



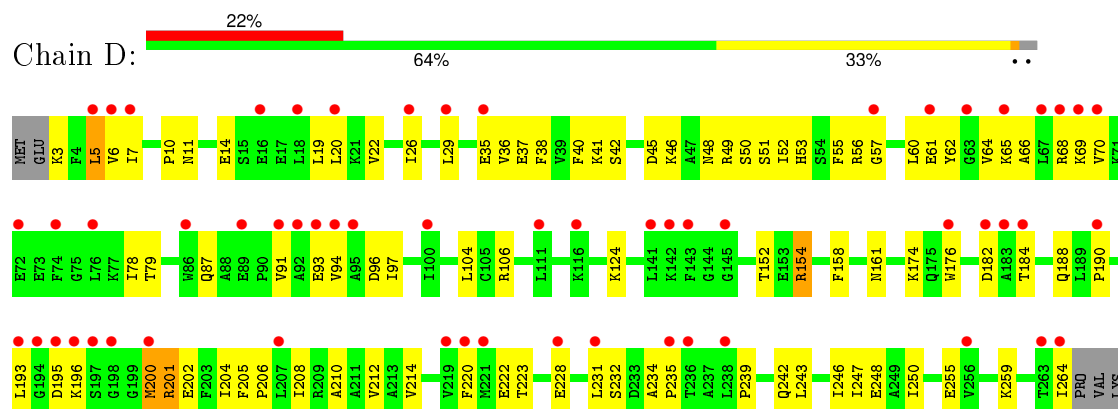
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



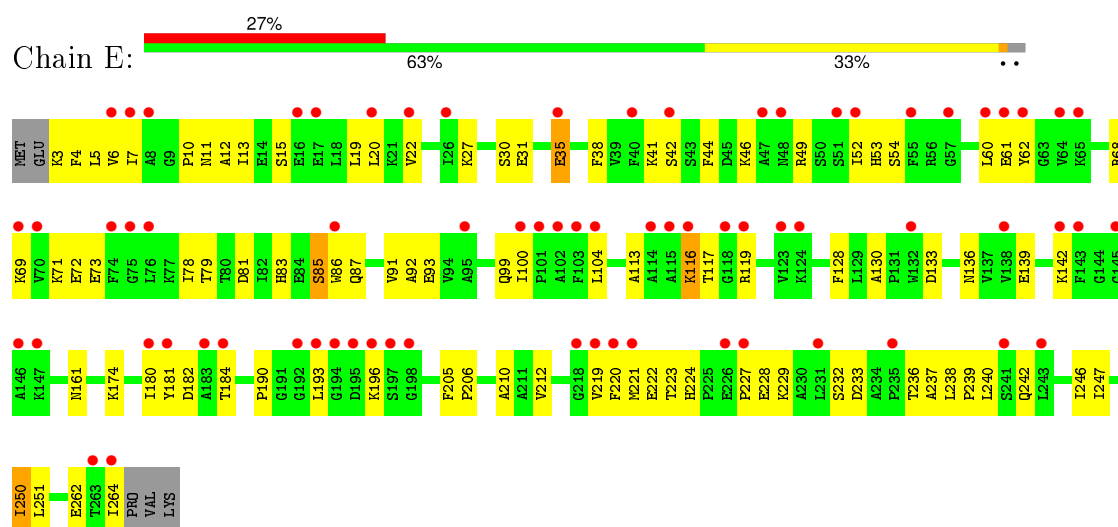
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



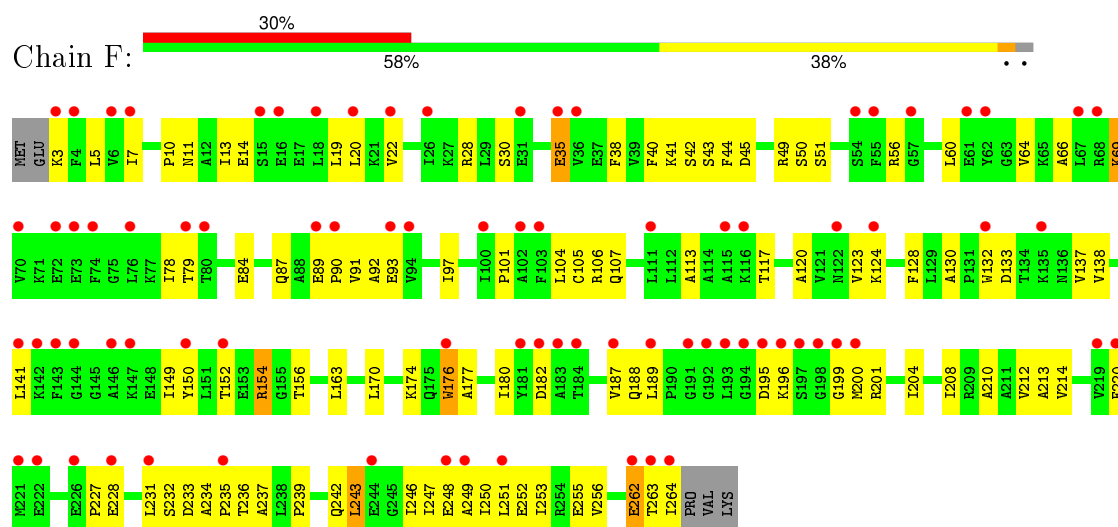
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



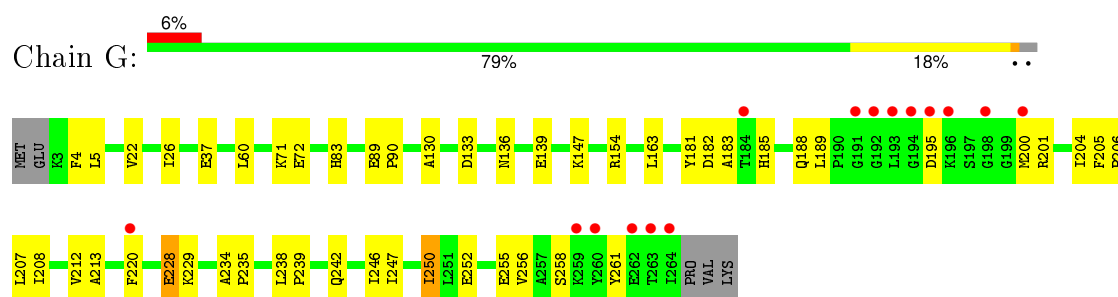
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



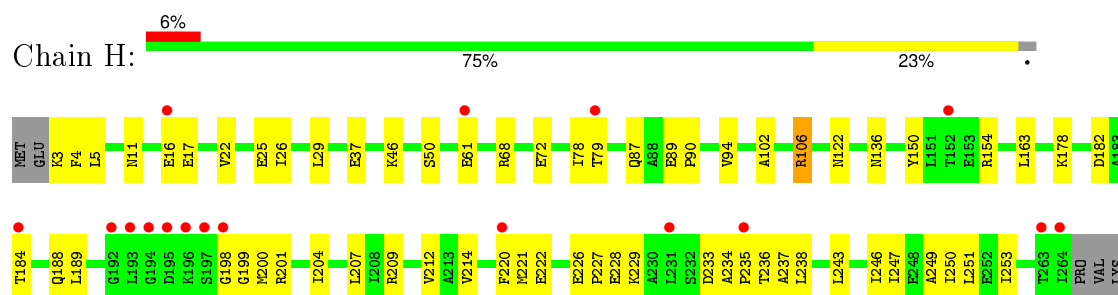
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



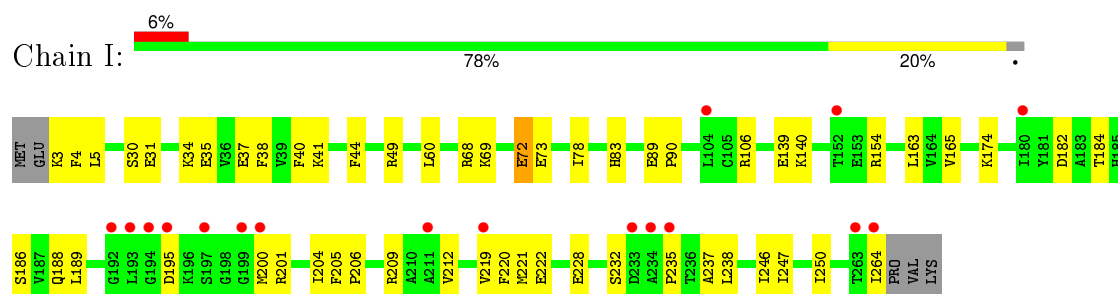
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



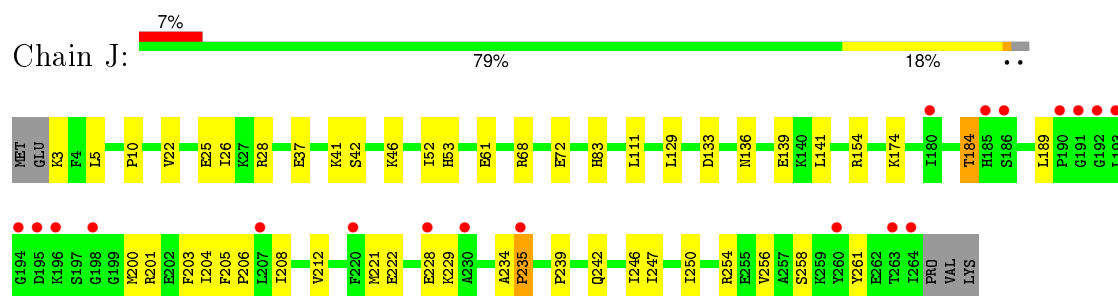
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



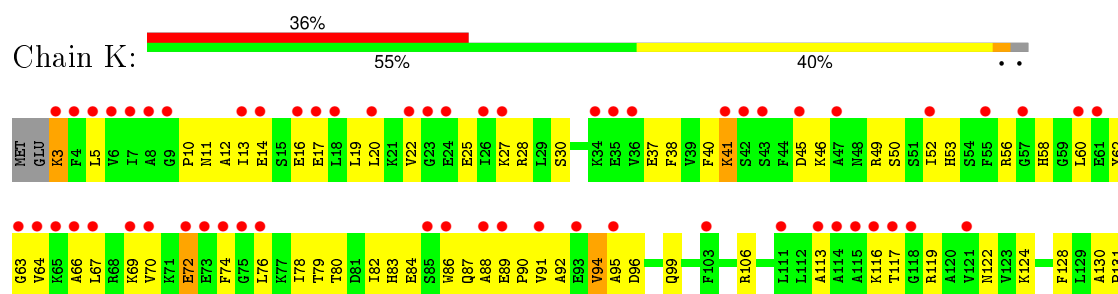
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

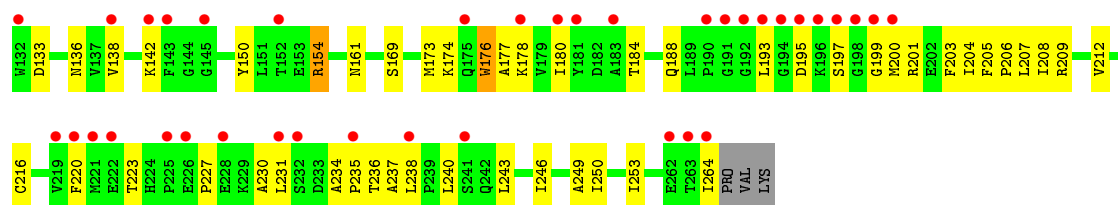


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

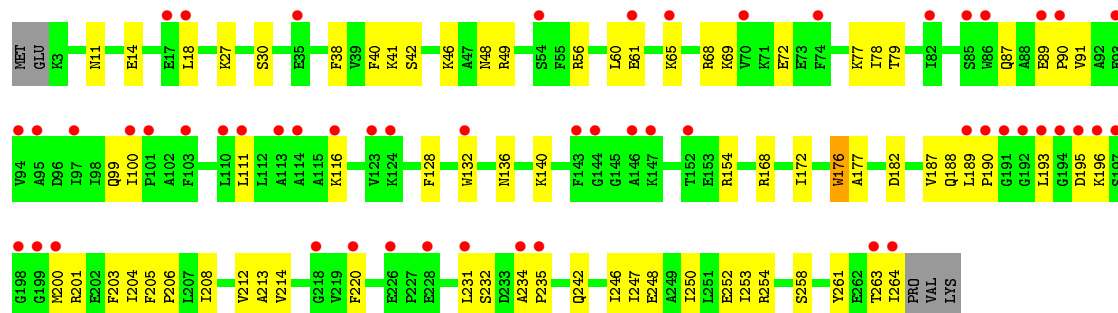


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase





• 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	76.38Å 198.53Å 125.83Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	29.79 – 2.10 29.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.79-2.10) 94.6 (29.79-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.261 0.214 , 0.260	Depositor DCC
R_{free} test set	20580 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	5 of 215998 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26573	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 19.98 % 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 9.6054e-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, 0.375 respectively for untwinned datasets, and 0.333, 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: 1NT, A5P, 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	0.42	1/2097 (0.0%)	0.61	0/2830
1	B	0.39	0/2097	0.62	0/2830
1	C	0.36	1/2097 (0.0%)	0.55	0/2830
1	D	0.32	0/2097	0.55	0/2830
1	E	0.35	1/2097 (0.0%)	0.52	0/2830
1	F	0.30	0/2097	0.52	0/2830
1	G	0.39	1/2097 (0.0%)	0.60	0/2830
1	H	0.38	0/2097	0.61	0/2830
1	I	0.42	1/2097 (0.0%)	0.60	0/2830
1	J	0.37	0/2097	0.60	0/2830
1	K	0.33	1/2097 (0.0%)	0.52	0/2830
1	L	0.32	0/2097	0.54	0/2830
All	All	0.36	6/25164 (0.0%)	0.57	0/33960

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	GLU	CD-OE2	7.44	1.33	1.25
1	E	72	GLU	CD-OE2	7.12	1.33	1.25
1	K	72	GLU	CD-OE2	7.11	1.33	1.25
1	G	72	GLU	CD-OE2	6.99	1.33	1.25
1	C	72	GLU	CD-OE2	6.97	1.33	1.25
1	I	72	GLU	CD-OE2	6.87	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 ⓘ

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	2055	0	2095	34	0
1	B	2055	0	2095	58	0
1	C	2055	0	2095	62	0
1	D	2055	0	2095	75	0
1	E	2055	0	2095	78	0
1	F	2055	0	2095	101	0
1	G	2055	0	2095	45	0
1	H	2055	0	2095	69	0
1	I	2055	0	2095	53	0
1	J	2055	0	2095	56	0
1	K	2055	0	2095	108	0
1	L	2055	0	2095	66	0
2	A	10	0	2	2	0
2	B	10	0	2	4	0
2	C	10	0	2	2	0
2	E	10	0	2	1	0
2	F	10	0	2	2	0
2	G	10	0	2	1	0
2	H	10	0	2	5	0
2	I	10	0	2	5	0
2	J	10	0	2	3	0
2	K	10	0	2	2	0
2	L	10	0	2	2	0
3	A	14	0	10	2	0
3	B	14	0	10	6	0
3	C	14	0	10	3	0
3	E	14	0	10	0	0
3	F	14	0	10	4	0
3	G	14	0	10	3	0
3	H	14	0	10	3	0
3	I	14	0	10	3	0
3	J	14	0	10	2	0
3	K	14	0	10	1	0
3	L	14	0	10	1	0
4	D	25	0	13	4	0
5	A	194	0	0	4	0
5	B	197	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	108	0	0	6	0
5	D	88	0	0	10	0
5	E	71	0	0	6	0
5	F	55	0	0	5	0
5	G	177	0	0	8	0
5	H	191	0	0	12	0
5	I	191	0	0	12	0
5	J	184	0	0	10	0
5	K	56	0	0	12	0
5	L	112	0	0	9	0
All	All	26573	0	25285	794	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 16.

All (794) 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:H:184:THR:HG21	1:H:222:GLU:H	1.15	1.12
1:B:184:THR:HG21	1:B:222:GLU:H	1.17	1.06
1:B:151:LEU:HB3	1:B:173:MET:HE1	1.37	1.04
1:I:154:ARG:HH22	1:I:188:GLN:NE2	1.62	0.98
1:D:212:VAL:HG11	1:D:250:ILE:HG23	1.47	0.96
1:C:11:ASN:HD21	1:C:46:LYS:HE2	1.31	0.94
1:I:154:ARG:NH2	1:I:188:GLN:HE21	1.64	0.94
1:I:174:LYS:HG3	1:I:264:ILE:HG12	1.53	0.90
1:H:184:THR:HG22	5:H:402:HOH:O	1.71	0.89
1:E:184:THR:HG21	1:E:222:GLU:H	1.37	0.88
1:J:184:THR:HG21	1:J:222:GLU:H	1.36	0.88
1:I:154:ARG:HH22	1:I:188:GLN:HE21	0.88	0.87
1:K:161:ASN:HD21	1:L:132:TRP:HE1	1.19	0.85
1:F:188:GLN:HA	1:F:199:GLY:HA2	1.60	0.84
1:C:174:LYS:HG3	1:C:264:ILE:HD13	1.57	0.84
1:C:49:ARG:HA	3:C:269:A5P:H51	1.58	0.83
1:B:154:ARG:HH22	1:B:188:GLN:NE2	1.77	0.83
2:J:268:PEP:C3	3:J:269:A5P:H12	2.09	0.82
1:E:161:ASN:HD21	1:F:132:TRP:HE1	1.23	0.82
1:K:227:PRO:HB3	1:K:237:ALA:HB3	1.59	0.81
1:D:174:LYS:HG2	1:D:264:ILE:HD13	1.62	0.81
3:G:269:A5P:H52	1:H:106:ARG:NH2	1.95	0.81
1:L:154:ARG:HH22	1:L:188:GLN:NE2	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:VAL:HG11	1:K:250:ILE:HG23	1.62	0.80
1:B:37:GLU:HG3	5:B:463:HOH:O	1.80	0.80
1:F:10:PRO:HD3	1:F:22:VAL:HG11	1.65	0.79
1:E:49:ARG:HE	1:E:54:SER:HB3	1.47	0.79
1:H:154:ARG:HH22	1:H:188:GLN:HE21	1.30	0.79
1:G:154:ARG:HH22	1:G:188:GLN:NE2	1.82	0.78
1:K:64:VAL:HG13	1:K:94:VAL:HG11	1.65	0.78
1:D:40:PHE:HB3	1:D:78:ILE:HD13	1.63	0.78
1:J:68:ARG:O	1:J:72:GLU:HG3	1.84	0.78
1:G:71:LYS:HE2	5:G:442:HOH:O	1.84	0.77
1:E:227:PRO:HB3	1:E:237:ALA:HB3	1.66	0.77
1:D:223:THR:HG21	1:D:243:LEU:HD11	1.67	0.76
2:I:268:PEP:C2	3:I:269:A5P:H12	2.15	0.76
3:G:269:A5P:H52	1:H:106:ARG:HH22	1.49	0.76
2:I:268:PEP:C3	3:I:269:A5P:H12	2.16	0.76
2:J:268:PEP:C2	3:J:269:A5P:H12	2.16	0.75
1:B:184:THR:CG2	1:B:222:GLU:H	1.98	0.75
1:E:11:ASN:HD21	1:E:46:LYS:HE3	1.51	0.75
1:F:256:VAL:HG21	1:G:256:VAL:HG11	1.68	0.75
1:A:65:LYS:HE3	5:G:441:HOH:O	1.84	0.75
1:I:69:LYS:HE3	1:I:73:GLU:OE1	1.87	0.75
1:D:154:ARG:HH22	1:D:188:GLN:HE21	1.35	0.74
1:E:35:GLU:H	1:E:35:GLU:CD	1.91	0.74
1:B:151:LEU:HD13	1:B:173:MET:HE2	1.69	0.74
1:H:184:THR:CG2	1:H:222:GLU:H	1.98	0.73
1:K:136:ASN:HD21	1:L:195:ASP:HA	1.52	0.73
1:E:68:ARG:NH1	1:E:68:ARG:HB2	2.02	0.73
1:G:238:LEU:HD21	1:G:246:ILE:HD12	1.70	0.73
1:K:138:VAL:O	1:K:142:LYS:HG2	1.88	0.73
1:J:154:ARG:HD2	2:J:268:PEP:O3P	1.89	0.73
1:H:184:THR:HG21	1:H:222:GLU:N	1.99	0.73
1:C:11:ASN:ND2	1:C:46:LYS:HE2	2.02	0.72
1:H:235:PRO:HA	5:H:450:HOH:O	1.89	0.72
1:K:205:PHE:HB3	1:K:206:PRO:HD3	1.70	0.72
2:B:268:PEP:C3	3:B:269:A5P:H12	2.19	0.72
1:E:11:ASN:ND2	1:E:46:LYS:HE3	2.04	0.72
1:I:189:LEU:HD11	1:I:200:MET:HE3	1.72	0.72
2:B:268:PEP:C2	3:B:269:A5P:H12	2.19	0.72
1:A:182:ASP:HA	1:A:220:PHE:HB3	1.70	0.71
1:F:66:ALA:HA	5:F:323:HOH:O	1.90	0.71
1:G:154:ARG:HD2	2:G:268:PEP:O3P	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:ILE:H	1:F:7:ILE:HD12	1.56	0.70
1:G:139:GLU:HG3	5:G:403:HOH:O	1.90	0.70
1:F:7:ILE:N	1:F:7:ILE:HD12	2.05	0.70
1:K:246:ILE:O	1:K:250:ILE:HG13	1.91	0.70
1:J:246:ILE:O	1:J:250:ILE:HG23	1.92	0.70
1:G:154:ARG:HH22	1:G:188:GLN:HE21	1.37	0.70
1:A:228:GLU:H	1:A:228:GLU:CD	1.95	0.70
1:D:205:PHE:HB3	1:D:206:PRO:HD3	1.73	0.70
1:K:113:ALA:HA	1:K:116:LYS:HD2	1.74	0.70
1:B:65:LYS:HA	1:B:65:LYS:HE3	1.73	0.69
1:C:189:LEU:HD21	1:C:200:MET:CE	2.23	0.69
1:J:174:LYS:HB2	5:J:403:HOH:O	1.91	0.69
1:F:212:VAL:HG23	1:F:253:ILE:HG21	1.73	0.69
1:B:134:THR:HG21	1:B:173:MET:CE	2.24	0.68
1:F:69:LYS:HE3	1:F:69:LYS:HA	1.76	0.68
1:F:234:ALA:HB3	1:F:235:PRO:HD3	1.76	0.68
1:J:41:LYS:HZ3	1:J:222:GLU:HG2	1.59	0.67
1:G:182:ASP:HA	1:G:220:PHE:HB3	1.75	0.67
1:H:154:ARG:HD2	2:H:268:PEP:O3P	1.94	0.67
1:L:204:ILE:O	1:L:208:ILE:HG13	1.94	0.67
1:K:10:PRO:HD3	1:K:22:VAL:HG11	1.77	0.67
1:A:41:LYS:HD2	1:A:42:SER:N	2.10	0.67
1:L:248:GLU:O	1:L:252:GLU:HG3	1.94	0.67
1:H:184:THR:HG23	1:H:221:MET:HA	1.75	0.67
1:L:190:PRO:HG3	5:L:292:HOH:O	1.94	0.67
1:E:3:LYS:HG3	1:E:35:GLU:O	1.95	0.67
1:J:201:ARG:NH1	1:J:201:ARG:HB2	2.09	0.67
1:I:184:THR:HG21	1:I:222:GLU:H	1.59	0.67
1:G:246:ILE:O	1:G:250:ILE:HG23	1.94	0.66
1:F:246:ILE:O	1:F:250:ILE:HG13	1.95	0.66
1:D:234:ALA:HB3	1:D:235:PRO:HD3	1.77	0.66
5:I:416:HOH:O	1:J:53:HIS:HD2	1.77	0.66
1:K:223:THR:HG21	1:K:243:LEU:HD22	1.77	0.66
1:C:22:VAL:O	1:C:26:ILE:HG12	1.96	0.66
1:K:52:ILE:HB	1:L:140:LYS:HG2	1.77	0.65
1:C:154:ARG:HD2	2:C:268:PEP:O3P	1.94	0.65
1:D:210:ALA:O	1:D:214:VAL:HG23	1.96	0.65
1:I:235:PRO:HA	5:I:335:HOH:O	1.97	0.65
1:F:123:VAL:HG11	1:F:137:VAL:HG11	1.78	0.65
1:I:40:PHE:HB3	1:I:78:ILE:HD13	1.79	0.65
1:H:22:VAL:O	1:H:26:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:TYR:CD1	1:K:178:LYS:HB2	2.32	0.65
1:D:14:GLU:HG2	1:D:231:LEU:HD12	1.78	0.64
1:A:189:LEU:HD21	1:A:200:MET:CE	2.27	0.64
1:E:61:GLU:HG2	1:E:62:TYR:H	1.60	0.64
1:E:68:ARG:HB2	1:E:68:ARG:HH11	1.63	0.64
1:K:19:LEU:HD22	1:K:66:ALA:HB1	1.78	0.64
1:B:184:THR:HG21	1:B:222:GLU:N	2.03	0.63
1:D:45:ASP:HA	1:D:56:ARG:O	1.98	0.63
1:D:19:LEU:HD12	1:D:66:ALA:HB1	1.80	0.63
1:A:200:MET:HG2	5:A:443:HOH:O	1.98	0.63
1:E:5:LEU:HD23	1:E:6:VAL:N	2.14	0.63
1:L:40:PHE:HB3	1:L:78:ILE:HD13	1.81	0.63
1:A:205:PHE:HB3	1:A:206:PRO:HD3	1.81	0.63
1:C:182:ASP:HA	1:C:220:PHE:HB3	1.80	0.62
1:I:189:LEU:HD21	1:I:200:MET:HE3	1.80	0.62
1:E:212:VAL:HG11	1:E:250:ILE:HB	1.79	0.62
1:B:154:ARG:HD2	2:B:268:PEP:O3P	1.98	0.62
1:H:16:GLU:HG3	1:H:17:GLU:N	2.15	0.62
1:G:154:ARG:NH2	1:G:188:GLN:HE21	1.97	0.62
1:K:84:GLU:HG3	5:K:310:HOH:O	1.98	0.62
1:L:263:THR:HG22	1:L:264:ILE:HG13	1.80	0.62
1:I:264:ILE:HD13	5:I:441:HOH:O	1.98	0.62
1:F:14:GLU:HG2	1:F:231:LEU:HD12	1.81	0.62
1:F:97:ILE:HG12	1:F:120:ALA:HB3	1.82	0.62
1:B:154:ARG:HH22	1:B:188:GLN:HE21	1.45	0.62
2:H:268:PEP:C2	3:H:269:A5P:H12	2.30	0.62
1:D:154:ARG:HH22	1:D:188:GLN:NE2	1.98	0.62
1:K:88:ALA:HB3	5:K:309:HOH:O	2.00	0.62
1:A:201:ARG:HG3	1:A:204:ILE:HD12	1.81	0.61
1:K:174:LYS:HE2	5:K:325:HOH:O	2.01	0.61
1:H:234:ALA:HA	5:H:274:HOH:O	2.00	0.61
1:E:237:ALA:HB2	5:E:334:HOH:O	2.00	0.61
4:D:268:1NT:HI31	4:D:268:1NT:O2P	1.98	0.61
1:D:243:LEU:O	1:D:247:ILE:HG13	2.01	0.61
1:G:189:LEU:HD21	1:G:200:MET:CE	2.31	0.61
1:F:101:PRO:HG2	1:F:104:LEU:HD12	1.82	0.61
1:B:201:ARG:HG3	1:B:204:ILE:HD12	1.83	0.61
1:L:77:LYS:HG3	5:L:310:HOH:O	2.00	0.61
1:I:83:HIS:HD2	5:J:289:HOH:O	1.82	0.60
1:J:189:LEU:HD21	1:J:200:MET:CE	2.30	0.60
1:D:97:ILE:N	1:D:97:ILE:HD12	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ARG:HA	3:F:269:A5P:H51	1.81	0.60
1:C:83:HIS:HD2	5:D:293:HOH:O	1.83	0.60
1:C:187:VAL:HG21	1:C:204:ILE:HG12	1.83	0.60
1:F:212:VAL:HG23	1:F:253:ILE:CG2	2.31	0.60
1:A:3:LYS:HD2	1:A:35:GLU:O	2.02	0.60
1:F:180:ILE:HD12	1:F:180:ILE:N	2.17	0.60
1:F:212:VAL:HG11	1:F:250:ILE:HG23	1.83	0.60
1:H:228:GLU:HG3	1:H:229:LYS:HG3	1.82	0.60
1:J:234:ALA:N	1:J:235:PRO:HD2	2.16	0.60
1:J:28:ARG:HD3	5:J:448:HOH:O	2.00	0.60
1:E:246:ILE:O	1:E:250:ILE:HG23	2.02	0.60
1:L:11:ASN:HD22	1:L:232:SER:HB3	1.66	0.59
1:F:124:LYS:HD3	1:F:152:THR:HB	1.84	0.59
1:H:201:ARG:HG3	1:H:204:ILE:HD12	1.84	0.59
1:J:189:LEU:HD21	1:J:200:MET:HE2	1.84	0.59
1:D:61:GLU:HB3	5:D:310:HOH:O	2.02	0.59
1:E:15:SER:O	1:E:19:LEU:HD13	2.02	0.59
1:E:174:LYS:HG3	1:E:264:ILE:HG21	1.84	0.59
1:K:150:TYR:HD1	1:K:178:LYS:HB2	1.68	0.59
1:E:41:LYS:C	1:E:41:LYS:HD3	2.23	0.59
1:F:247:ILE:O	1:F:251:LEU:HG	2.02	0.59
1:K:17:GLU:HG3	5:K:319:HOH:O	2.02	0.59
1:I:184:THR:HB	5:I:412:HOH:O	2.03	0.59
1:K:195:ASP:HA	1:L:136:ASN:HD21	1.66	0.59
1:I:4:PHE:CZ	1:I:219:VAL:HG23	2.38	0.59
1:J:46:LYS:HA	1:J:46:LYS:HE2	1.84	0.59
1:A:11:ASN:HD21	1:A:46:LYS:HE2	1.68	0.59
1:I:189:LEU:HD21	1:I:200:MET:CE	2.33	0.58
1:L:11:ASN:HD21	1:L:46:LYS:HE3	1.67	0.58
1:K:3:LYS:HE3	1:K:3:LYS:N	2.17	0.58
1:I:106:ARG:HA	5:I:306:HOH:O	2.03	0.58
1:E:184:THR:HG21	1:E:222:GLU:N	2.13	0.58
1:A:11:ASN:HD21	1:A:46:LYS:CE	2.16	0.58
1:I:182:ASP:HA	1:I:220:PHE:HB3	1.85	0.58
1:G:228:GLU:H	1:G:228:GLU:CD	2.05	0.58
1:C:43:SER:HB2	1:C:46:LYS:HZ1	1.68	0.58
1:H:154:ARG:HH22	1:H:188:GLN:NE2	2.01	0.58
1:E:69:LYS:NZ	1:E:73:GLU:HB2	2.18	0.58
1:I:209:ARG:HH12	1:L:214:VAL:HA	1.68	0.58
1:K:27:LYS:HA	1:K:76:LEU:HD21	1.85	0.58
1:F:150:TYR:CD1	1:F:180:ILE:HD11	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:ASP:HB3	1:F:236:THR:OG1	2.03	0.58
1:B:228:GLU:H	1:B:228:GLU:CD	2.07	0.58
1:E:52:ILE:HG23	1:E:53:HIS:CD2	2.38	0.58
1:E:11:ASN:HD22	1:E:232:SER:HB3	1.67	0.58
1:C:136:ASN:HD21	1:D:195:ASP:HA	1.67	0.58
1:F:189:LEU:HD11	1:F:200:MET:CE	2.34	0.58
1:C:41:LYS:HD2	1:C:42:SER:N	2.19	0.58
1:H:243:LEU:O	1:H:247:ILE:HG12	2.04	0.58
1:G:189:LEU:HD21	1:G:200:MET:HE2	1.85	0.57
1:J:41:LYS:HD2	5:J:447:HOH:O	2.04	0.57
1:L:154:ARG:HD2	2:L:268:PEP:O3P	2.04	0.57
1:L:100:ILE:HG12	1:L:111:LEU:HD23	1.86	0.57
1:D:242:GLN:O	1:D:246:ILE:HD13	2.04	0.57
1:B:161:ASN:HA	1:B:190:PRO:HG2	1.85	0.57
1:I:68:ARG:O	1:I:72:GLU:HG3	2.05	0.57
1:H:154:ARG:NH2	1:H:188:GLN:HE21	2.02	0.57
1:E:41:LYS:HD3	1:E:42:SER:N	2.19	0.57
1:D:228:GLU:HB3	5:D:346:HOH:O	2.03	0.57
1:F:3:LYS:HB2	1:F:35:GLU:O	2.04	0.57
1:C:43:SER:HB2	1:C:46:LYS:NZ	2.20	0.57
1:E:68:ARG:CB	1:E:68:ARG:HH11	2.18	0.57
1:A:189:LEU:HD21	1:A:200:MET:HE2	1.86	0.57
1:D:3:LYS:HB2	5:D:339:HOH:O	2.03	0.57
1:E:49:ARG:HE	1:E:54:SER:CB	2.18	0.57
1:J:41:LYS:NZ	1:J:222:GLU:HG2	2.19	0.57
5:A:424:HOH:O	1:B:83:HIS:HD2	1.87	0.57
1:F:263:THR:HG22	1:F:264:ILE:H	1.68	0.57
1:C:106:ARG:HA	5:C:376:HOH:O	2.04	0.57
1:F:45:ASP:HA	1:F:56:ARG:O	2.05	0.57
1:F:45:ASP:OD1	1:F:56:ARG:HB3	2.05	0.57
1:G:229:LYS:HE2	5:G:414:HOH:O	2.04	0.56
1:I:209:ARG:NH1	1:L:213:ALA:O	2.38	0.56
1:J:239:PRO:HG2	1:J:242:GLN:NE2	2.21	0.56
1:D:41:LYS:HD3	1:D:42:SER:N	2.20	0.56
1:H:201:ARG:HA	1:H:204:ILE:HG13	1.87	0.56
1:E:250:ILE:C	1:E:250:ILE:HD12	2.26	0.56
1:H:11:ASN:HD21	1:H:46:LYS:NZ	2.01	0.56
1:K:188:GLN:HB3	1:K:236:THR:HG21	1.87	0.56
1:A:154:ARG:HD2	2:A:268:PEP:O3P	2.05	0.56
1:H:249:ALA:O	1:H:253:ILE:HG12	2.04	0.56
1:G:204:ILE:O	1:G:208:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:ALA:HB2	1:K:46:LYS:HD3	1.87	0.56
1:H:228:GLU:HG2	5:H:403:HOH:O	2.06	0.56
1:E:223:THR:OG1	1:E:240:LEU:HA	2.05	0.56
1:D:20:LEU:HD23	1:D:70:VAL:HG22	1.87	0.56
1:B:240:LEU:O	1:B:243:LEU:HD13	2.06	0.56
1:C:14:GLU:OE2	1:C:231:LEU:HG	2.06	0.56
1:F:40:PHE:HB3	1:F:78:ILE:HD13	1.86	0.56
1:K:204:ILE:O	1:K:208:ILE:HG13	2.06	0.56
1:K:136:ASN:ND2	1:L:195:ASP:HA	2.21	0.56
1:F:200:MET:HE3	5:F:288:HOH:O	2.05	0.56
1:H:182:ASP:HA	1:H:220:PHE:HB3	1.88	0.56
1:I:31:GLU:O	1:I:34:LYS:HE3	2.05	0.56
1:F:154:ARG:HD2	2:F:268:PEP:O3P	2.06	0.56
1:H:237:ALA:HB3	5:H:274:HOH:O	2.06	0.56
1:H:189:LEU:HD11	1:H:200:MET:CE	2.36	0.56
1:E:228:GLU:HG3	1:E:229:LYS:HG3	1.88	0.56
1:C:100:ILE:HG13	1:C:111:LEU:HD23	1.87	0.56
1:A:41:LYS:HB2	1:A:79:THR:CG2	2.36	0.55
1:H:201:ARG:HH12	1:H:227:PRO:HB2	1.72	0.55
1:H:201:ARG:NH2	1:H:234:ALA:O	2.38	0.55
1:E:242:GLN:O	1:E:246:ILE:HD13	2.06	0.55
1:B:237:ALA:HB3	5:B:301:HOH:O	2.04	0.55
1:B:212:VAL:HG11	1:B:250:ILE:HG23	1.87	0.55
1:K:70:VAL:HG13	1:K:78:ILE:HD11	1.88	0.55
1:H:68:ARG:HH21	1:H:94:VAL:HG23	1.70	0.55
1:F:28:ARG:HG2	1:F:28:ARG:HH11	1.72	0.55
1:B:134:THR:HG21	1:B:173:MET:HE3	1.88	0.55
1:J:184:THR:CG2	1:J:222:GLU:H	2.13	0.55
1:F:189:LEU:N	1:F:189:LEU:HD12	2.22	0.55
1:E:182:ASP:HA	1:E:220:PHE:HB3	1.89	0.55
1:C:11:ASN:ND2	1:C:232:SER:OG	2.39	0.55
1:H:198:GLY:HA2	1:H:235:PRO:HG3	1.88	0.55
1:L:87:GLN:O	1:L:91:VAL:HG23	2.05	0.55
1:B:182:ASP:HA	1:B:220:PHE:HB3	1.88	0.55
1:D:64:VAL:HG13	1:D:94:VAL:CG1	2.37	0.55
1:E:116:LYS:NZ	1:E:116:LYS:HB2	2.21	0.55
1:E:20:LEU:HD21	1:E:69:LYS:HG3	1.88	0.55
1:F:106:ARG:HG3	1:F:106:ARG:HH11	1.71	0.55
1:B:49:ARG:NH2	1:B:231:LEU:O	2.40	0.54
1:A:235:PRO:HA	5:A:436:HOH:O	2.07	0.54
1:K:63:GLY:O	1:K:67:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:128:PHE:HB3	5:L:282:HOH:O	2.06	0.54
1:F:91:VAL:C	1:F:93:GLU:H	2.11	0.54
1:K:227:PRO:HB3	1:K:237:ALA:CB	2.34	0.54
1:K:60:LEU:HD23	1:K:60:LEU:C	2.27	0.54
1:F:138:VAL:HG11	1:F:176:TRP:O	2.07	0.54
3:G:269:A5P:C5	1:H:106:ARG:HH22	2.20	0.54
1:F:249:ALA:O	1:F:253:ILE:HD13	2.08	0.54
1:D:19:LEU:HD22	1:D:40:PHE:HE2	1.73	0.54
1:K:52:ILE:HG23	1:K:53:HIS:CD2	2.42	0.54
1:F:243:LEU:O	1:F:247:ILE:HG13	2.08	0.54
1:G:183:ALA:HB2	1:G:208:ILE:HG12	1.90	0.54
1:H:68:ARG:HE	1:H:94:VAL:CG2	2.21	0.54
1:E:130:ALA:HB3	1:E:133:ASP:OD2	2.07	0.54
1:K:83:HIS:HD2	5:K:305:HOH:O	1.91	0.54
1:G:238:LEU:HD21	1:G:246:ILE:CD1	2.38	0.54
1:C:228:GLU:HG3	1:C:229:LYS:HG3	1.89	0.54
1:L:41:LYS:HD3	1:L:42:SER:N	2.23	0.53
1:C:20:LEU:HB3	5:C:362:HOH:O	2.07	0.53
1:E:239:PRO:HG2	1:E:242:GLN:NE2	2.24	0.53
1:L:11:ASN:ND2	1:L:46:LYS:HE3	2.22	0.53
1:E:87:GLN:O	1:E:91:VAL:HG22	2.09	0.53
1:J:184:THR:HB	5:J:399:HOH:O	2.06	0.53
1:D:264:ILE:HD12	5:D:342:HOH:O	2.07	0.53
1:K:113:ALA:O	1:K:116:LYS:HG2	2.09	0.53
1:K:41:LYS:HB2	1:K:79:THR:CG2	2.39	0.53
1:B:151:LEU:HD13	1:B:173:MET:CE	2.37	0.53
1:H:68:ARG:HH21	1:H:94:VAL:CG2	2.21	0.53
1:C:234:ALA:HB3	1:C:235:PRO:HD3	1.90	0.53
1:J:41:LYS:HG2	1:J:42:SER:N	2.24	0.53
1:F:49:ARG:HE	3:F:269:A5P:H52	1.72	0.53
1:J:3:LYS:N	5:J:368:HOH:O	2.42	0.53
1:L:49:ARG:HD2	3:L:269:A5P:O4	2.08	0.53
1:L:68:ARG:O	1:L:72:GLU:HG3	2.08	0.53
1:G:234:ALA:N	1:G:235:PRO:HD2	2.24	0.53
1:C:189:LEU:HD21	1:C:200:MET:HE3	1.89	0.53
1:L:46:LYS:HB2	1:L:56:ARG:HA	1.90	0.53
1:K:200:MET:HB3	1:K:203:PHE:HD2	1.74	0.53
1:D:51:SER:HB2	1:D:195:ASP:HB2	1.90	0.52
1:F:113:ALA:O	1:F:117:THR:HG23	2.09	0.52
1:F:7:ILE:H	1:F:7:ILE:CD1	2.21	0.52
1:A:41:LYS:HB2	1:A:79:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:ARG:HE	1:H:94:VAL:HG22	1.75	0.52
1:L:41:LYS:C	1:L:41:LYS:HD3	2.29	0.52
1:H:238:LEU:HD21	1:H:246:ILE:CD1	2.39	0.52
1:D:68:ARG:HH21	1:D:93:GLU:HB3	1.74	0.52
1:I:247:ILE:O	1:I:250:ILE:HG13	2.09	0.52
1:F:182:ASP:HA	1:F:220:PHE:HB3	1.92	0.52
1:E:60:LEU:HD23	1:E:60:LEU:C	2.29	0.52
1:B:233:ASP:OD2	3:B:269:A5P:HC3	2.10	0.52
1:D:182:ASP:HA	1:D:220:PHE:HB3	1.92	0.52
1:B:134:THR:HG21	1:B:173:MET:HE2	1.91	0.52
1:K:91:VAL:O	1:K:94:VAL:HG12	2.09	0.52
1:C:20:LEU:HD12	5:C:359:HOH:O	2.07	0.52
1:B:263:THR:HG22	1:B:264:ILE:HG13	1.91	0.52
1:L:182:ASP:HA	1:L:220:PHE:HB3	1.92	0.52
1:A:136:ASN:HB3	1:B:50:SER:O	2.09	0.52
1:J:208:ILE:O	1:J:212:VAL:HG23	2.10	0.52
1:K:180:ILE:N	1:K:180:ILE:HD12	2.24	0.52
1:G:130:ALA:HB3	1:G:133:ASP:OD2	2.09	0.52
1:C:49:ARG:NE	3:C:269:A5P:H52	2.24	0.52
1:H:247:ILE:O	1:H:250:ILE:HG12	2.10	0.52
1:E:113:ALA:O	1:E:117:THR:HG23	2.10	0.52
1:C:201:ARG:HG3	1:C:235:PRO:O	2.09	0.52
1:B:11:ASN:HD21	1:B:46:LYS:NZ	2.08	0.52
1:K:238:LEU:HD21	1:K:246:ILE:HD12	1.92	0.52
2:I:268:PEP:C1	3:I:269:A5P:H12	2.40	0.51
1:K:87:GLN:O	1:K:91:VAL:HG23	2.10	0.51
1:A:11:ASN:HD21	1:A:46:LYS:NZ	2.08	0.51
1:E:78:ILE:HG22	1:E:79:THR:N	2.25	0.51
1:L:154:ARG:HH22	1:L:188:GLN:HE22	1.55	0.51
1:D:20:LEU:HD21	1:D:69:LYS:HG3	1.91	0.51
1:C:41:LYS:HD2	1:C:42:SER:H	1.75	0.51
1:K:45:ASP:HA	1:K:56:ARG:O	2.09	0.51
1:H:233:ASP:OD2	3:H:269:A5P:HC3	2.09	0.51
1:G:250:ILE:HD12	1:G:250:ILE:C	2.31	0.51
1:K:113:ALA:HA	1:K:116:LYS:CD	2.40	0.51
1:A:46:LYS:CE	3:A:269:A5P:H11	2.40	0.51
1:H:4:PHE:CE2	1:H:250:ILE:HD12	2.44	0.51
1:F:263:THR:HG22	1:F:264:ILE:N	2.26	0.51
1:C:13:ILE:HD12	1:C:44:PHE:HA	1.92	0.51
1:L:154:ARG:HH22	1:L:188:GLN:HE21	1.55	0.51
1:K:40:PHE:HB3	1:K:78:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:LEU:H	1:K:19:LEU:HD12	1.75	0.51
1:K:67:LEU:HB3	1:K:78:ILE:HG21	1.92	0.51
1:I:205:PHE:HB3	1:I:206:PRO:HD3	1.93	0.51
1:D:60:LEU:HD23	1:D:60:LEU:O	2.10	0.51
1:K:16:GLU:O	1:K:20:LEU:HD13	2.10	0.51
1:K:19:LEU:N	1:K:19:LEU:HD12	2.25	0.51
1:L:203:PHE:C	1:L:206:PRO:HD2	2.31	0.51
1:G:136:ASN:HB3	1:H:50:SER:O	2.11	0.51
1:I:154:ARG:HD2	2:I:268:PEP:O3P	2.10	0.51
1:F:256:VAL:HG21	1:G:256:VAL:CG1	2.40	0.51
1:A:212:VAL:HG11	1:A:250:ILE:HG23	1.92	0.51
1:A:170:LEU:HB2	1:A:171:PRO:HD3	1.93	0.51
1:C:189:LEU:HD21	1:C:200:MET:HE2	1.92	0.51
1:J:200:MET:HA	5:J:428:HOH:O	2.10	0.51
1:K:58:HIS:HB2	1:K:62:TYR:CD2	2.46	0.51
1:E:128:PHE:HB3	5:E:272:HOH:O	2.11	0.51
1:E:104:LEU:HD11	1:F:107:GLN:NE2	2.26	0.51
1:E:262:GLU:OE2	1:H:209:ARG:NH2	2.44	0.51
1:K:150:TYR:CD1	1:K:180:ILE:HD11	2.46	0.50
1:H:68:ARG:O	1:H:72:GLU:HG3	2.11	0.50
1:C:204:ILE:O	1:C:208:ILE:HG13	2.12	0.50
1:H:189:LEU:HD12	5:H:441:HOH:O	2.11	0.50
1:E:3:LYS:NZ	1:E:35:GLU:HA	2.27	0.50
5:E:272:HOH:O	1:F:128:PHE:HB3	2.11	0.50
1:L:258:SER:HA	1:L:261:TYR:CD2	2.46	0.50
1:G:83:HIS:HD2	5:H:341:HOH:O	1.93	0.50
1:F:78:ILE:HG22	1:F:79:THR:N	2.26	0.50
1:H:189:LEU:HD11	1:H:200:MET:HE3	1.92	0.50
1:E:205:PHE:HB3	1:E:206:PRO:HD3	1.94	0.50
1:H:178:LYS:HD3	5:H:378:HOH:O	2.12	0.50
1:F:10:PRO:HG3	1:F:22:VAL:HG21	1.94	0.50
1:I:204:ILE:HD13	1:I:238:LEU:HD11	1.94	0.50
1:E:61:GLU:HG2	1:E:62:TYR:N	2.27	0.50
1:G:185:HIS:HB3	1:G:188:GLN:HE21	1.75	0.50
1:F:256:VAL:CG2	1:G:256:VAL:HG11	2.41	0.50
1:D:201:ARG:NH1	1:D:235:PRO:HA	2.27	0.50
1:H:250:ILE:HG13	1:H:251:LEU:N	2.26	0.50
1:B:234:ALA:HB3	1:B:235:PRO:HD3	1.92	0.50
1:A:83:HIS:HD2	5:B:282:HOH:O	1.94	0.50
1:D:26:ILE:HD12	1:D:40:PHE:CD1	2.46	0.49
1:F:170:LEU:O	1:F:174:LYS:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:GLU:HG3	5:H:410:HOH:O	2.11	0.49
1:K:14:GLU:HG2	1:K:231:LEU:HD12	1.93	0.49
1:F:201:ARG:HG3	1:F:204:ILE:HD12	1.93	0.49
1:B:41:LYS:C	1:B:41:LYS:HD3	2.32	0.49
1:F:156:THR:O	1:F:163:LEU:HA	2.12	0.49
1:H:201:ARG:HH21	1:H:236:THR:N	2.10	0.49
1:J:201:ARG:HG3	1:J:204:ILE:HD12	1.93	0.49
1:E:136:ASN:HB3	1:F:50:SER:O	2.12	0.49
1:F:101:PRO:CG	1:F:104:LEU:HD12	2.43	0.49
1:F:243:LEU:CD1	1:F:247:ILE:HD11	2.43	0.49
1:J:205:PHE:HB3	1:J:206:PRO:HD3	1.95	0.49
1:I:139:GLU:HB2	5:I:390:HOH:O	2.12	0.49
1:G:212:VAL:HG11	1:G:250:ILE:HB	1.94	0.49
1:J:258:SER:HA	1:J:261:TYR:CE2	2.47	0.49
1:K:13:ILE:HG23	1:K:19:LEU:HD11	1.94	0.49
2:A:268:PEP:O1P	2:A:268:PEP:H32	2.13	0.49
1:F:87:GLN:O	1:F:91:VAL:HG23	2.13	0.49
1:E:91:VAL:C	1:E:93:GLU:H	2.16	0.49
1:K:89:GLU:HG2	5:K:309:HOH:O	2.13	0.49
1:K:27:LYS:O	1:K:30:SER:HB3	2.13	0.49
1:B:243:LEU:N	1:B:243:LEU:HD12	2.27	0.49
1:B:22:VAL:O	1:B:26:ILE:HG12	2.13	0.49
2:L:268:PEP:O1P	2:L:268:PEP:H32	2.12	0.49
1:B:243:LEU:O	1:B:247:ILE:HG12	2.13	0.49
1:F:13:ILE:HG13	1:F:43:SER:O	2.13	0.49
1:L:27:LYS:O	1:L:30:SER:HB3	2.12	0.49
1:E:224:HIS:O	1:E:227:PRO:HD3	2.12	0.49
1:I:238:LEU:HD12	1:I:238:LEU:N	2.28	0.49
1:K:69:LYS:HG2	5:K:316:HOH:O	2.12	0.49
1:L:14:GLU:HG2	1:L:231:LEU:HD12	1.95	0.49
1:D:204:ILE:O	1:D:208:ILE:HG13	2.13	0.48
1:L:65:LYS:HG2	5:L:336:HOH:O	2.13	0.48
1:E:100:ILE:HD12	1:E:100:ILE:N	2.27	0.48
1:D:41:LYS:C	1:D:41:LYS:HD3	2.33	0.48
5:I:409:HOH:O	1:J:83:HIS:HD2	1.95	0.48
1:L:61:GLU:HG3	5:L:319:HOH:O	2.12	0.48
1:E:139:GLU:HA	1:E:142:LYS:NZ	2.28	0.48
1:K:25:GLU:OE1	1:K:28:ARG:HD3	2.13	0.48
2:I:268:PEP:O1P	2:I:268:PEP:H32	2.12	0.48
1:K:30:SER:HA	1:K:38:PHE:CE2	2.48	0.48
1:B:261:TYR:HD1	1:C:209:ARG:HH12	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:ARG:NE	3:F:269:A5P:H52	2.28	0.48
1:H:188:GLN:HA	1:H:199:GLY:HA2	1.95	0.48
2:F:268:PEP:H32	2:F:268:PEP:O1P	2.13	0.48
1:L:14:GLU:HG2	1:L:231:LEU:CD1	2.44	0.48
1:D:124:LYS:HD3	1:D:152:THR:HB	1.95	0.48
1:C:60:LEU:C	1:C:60:LEU:HD23	2.34	0.48
1:C:12:ALA:HB2	1:C:46:LYS:HZ3	1.78	0.48
1:D:26:ILE:HD12	1:D:40:PHE:HD1	1.78	0.48
1:I:212:VAL:HG21	1:I:250:ILE:HB	1.95	0.48
1:L:116:LYS:HD3	5:L:348:HOH:O	2.14	0.48
1:K:234:ALA:HB3	1:K:235:PRO:HD3	1.94	0.48
1:E:233:ASP:HB3	1:E:236:THR:OG1	2.14	0.48
1:B:49:ARG:HD2	3:B:269:A5P:O3P	2.14	0.48
1:C:107:GLN:OE1	1:D:48:ASN:HB3	2.13	0.48
1:D:96:ASP:HB2	1:D:97:ILE:HD12	1.95	0.48
1:J:25:GLU:HA	1:J:28:ARG:NH1	2.28	0.48
1:C:47:ALA:HB1	5:C:287:HOH:O	2.14	0.48
1:F:176:TRP:O	1:F:177:ALA:HB2	2.14	0.48
1:K:5:LEU:HD12	1:K:37:GLU:O	2.13	0.48
1:I:4:PHE:HZ	1:I:219:VAL:HG23	1.79	0.47
1:I:5:LEU:HD12	1:I:37:GLU:O	2.13	0.47
1:G:4:PHE:CE2	1:G:250:ILE:HD13	2.49	0.47
1:K:41:LYS:C	1:K:41:LYS:HD3	2.34	0.47
1:G:181:TYR:OH	1:G:207:LEU:HD23	2.13	0.47
1:H:238:LEU:HD21	1:H:246:ILE:HD12	1.96	0.47
1:K:249:ALA:O	1:K:253:ILE:HG12	2.14	0.47
1:B:17:GLU:HG3	5:B:454:HOH:O	2.13	0.47
1:E:83:HIS:HD2	5:E:308:HOH:O	1.96	0.47
1:G:60:LEU:C	1:G:60:LEU:HD23	2.35	0.47
1:D:193:LEU:HB2	1:D:196:LYS:O	2.14	0.47
1:D:19:LEU:HD22	1:D:40:PHE:CE2	2.49	0.47
1:I:201:ARG:HG3	1:I:204:ILE:HD12	1.97	0.47
1:K:223:THR:OG1	1:K:240:LEU:HA	2.14	0.47
1:F:262:GLU:HB2	5:F:317:HOH:O	2.14	0.47
1:K:64:VAL:HG13	1:K:94:VAL:CG1	2.42	0.47
1:K:3:LYS:CA	1:K:3:LYS:HE3	2.45	0.47
1:L:60:LEU:HD23	1:L:60:LEU:C	2.35	0.47
1:F:228:GLU:OE1	1:F:228:GLU:N	2.44	0.47
1:E:238:LEU:HD12	1:E:239:PRO:HD2	1.97	0.47
1:I:4:PHE:CE2	1:I:250:ILE:HD13	2.49	0.47
1:K:200:MET:HB3	1:K:203:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ALA:HB3	1:F:133:ASP:OD2	2.14	0.47
1:E:27:LYS:O	1:E:31:GLU:HG2	2.15	0.47
1:B:154:ARG:HH21	1:B:163:LEU:CD1	2.28	0.47
1:K:41:LYS:HB2	1:K:79:THR:HG23	1.96	0.47
1:K:188:GLN:HA	1:K:199:GLY:HA2	1.97	0.47
1:F:41:LYS:HD3	1:F:42:SER:N	2.29	0.47
1:A:234:ALA:N	1:A:235:PRO:HD2	2.30	0.47
1:B:263:THR:HA	5:B:448:HOH:O	2.15	0.47
1:K:154:ARG:HD2	2:K:268:PEP:O3P	2.14	0.47
1:A:60:LEU:HD23	1:A:60:LEU:C	2.35	0.47
1:B:78:ILE:HG22	1:B:79:THR:N	2.28	0.47
1:D:184:THR:HG21	1:D:222:GLU:H	1.80	0.47
1:L:168:ARG:O	1:L:172:ILE:HG13	2.15	0.47
1:E:49:ARG:NH1	1:E:232:SER:OG	2.47	0.47
1:K:130:ALA:HB3	1:K:133:ASP:OD2	2.15	0.47
1:E:12:ALA:HB1	5:E:310:HOH:O	2.13	0.47
1:J:201:ARG:CB	1:J:201:ARG:HH11	2.28	0.47
1:F:189:LEU:HD11	1:F:200:MET:HE3	1.97	0.47
1:C:195:ASP:OD1	1:C:196:LYS:HG2	2.15	0.47
1:K:176:TRP:O	1:K:177:ALA:HB2	2.14	0.47
1:E:184:THR:HG23	1:E:221:MET:HA	1.97	0.46
1:K:184:THR:O	1:K:236:THR:HB	2.15	0.46
1:C:14:GLU:OE1	1:C:18:LEU:HD22	2.15	0.46
1:E:262:GLU:CD	1:H:209:ARG:HH22	2.19	0.46
1:D:5:LEU:HD22	1:D:37:GLU:HB3	1.97	0.46
1:A:50:SER:O	1:B:136:ASN:HB3	2.15	0.46
1:A:129:LEU:HG	1:A:133:ASP:HB2	1.97	0.46
1:E:11:ASN:ND2	1:E:232:SER:HB3	2.29	0.46
1:E:247:ILE:O	1:E:250:ILE:HG13	2.16	0.46
1:K:11:ASN:HD21	1:K:46:LYS:HE2	1.79	0.46
1:L:234:ALA:HB3	1:L:235:PRO:HD3	1.97	0.46
1:I:49:ARG:NH1	1:I:232:SER:HB3	2.29	0.46
1:B:61:GLU:HG3	5:B:335:HOH:O	2.16	0.46
1:I:195:ASP:HA	1:J:136:ASN:HD21	1.80	0.46
1:A:49:ARG:NH1	1:A:232:SER:HB3	2.30	0.46
1:D:154:ARG:HD2	4:D:268:1NT:O3P	2.15	0.46
1:E:4:PHE:CE2	1:E:250:ILE:HD13	2.50	0.46
1:C:136:ASN:HB3	1:D:50:SER:O	2.15	0.46
1:H:212:VAL:HG11	1:H:250:ILE:HB	1.96	0.46
1:J:239:PRO:HG2	1:J:242:GLN:HE21	1.79	0.46
1:G:258:SER:HA	1:G:261:TYR:CE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:206:PRO:HA	1:K:209:ARG:HE	1.81	0.46
1:K:206:PRO:HA	1:K:209:ARG:HH21	1.80	0.46
1:K:122:ASN:HA	1:K:150:TYR:HB2	1.96	0.46
1:D:259:LYS:N	5:D:337:HOH:O	2.42	0.46
1:B:259:LYS:HB3	1:B:259:LYS:NZ	2.30	0.46
1:I:3:LYS:N	5:I:451:HOH:O	2.48	0.46
5:G:294:HOH:O	1:J:139:GLU:HB2	2.15	0.46
1:C:239:PRO:HG2	1:C:242:GLN:NE2	2.30	0.46
1:F:248:GLU:HG3	1:F:252:GLU:OE2	2.16	0.46
1:E:85:SER:O	1:E:87:GLN:N	2.49	0.46
1:B:184:THR:CG2	1:B:221:MET:HA	2.46	0.46
1:B:185:HIS:NE2	3:B:269:A5P:H11	2.31	0.46
1:F:20:LEU:HD21	1:F:69:LYS:HG3	1.97	0.46
1:F:106:ARG:NH1	1:F:106:ARG:HG3	2.30	0.46
1:J:129:LEU:HG	1:J:133:ASP:HB2	1.97	0.46
1:C:246:ILE:O	1:C:250:ILE:HG12	2.15	0.46
1:G:205:PHE:N	1:G:206:PRO:HD2	2.30	0.46
1:D:19:LEU:HD12	1:D:66:ALA:CB	2.46	0.46
1:J:201:ARG:NH1	1:J:201:ARG:CB	2.78	0.46
1:C:41:LYS:HE3	1:C:220:PHE:HZ	1.81	0.46
1:L:128:PHE:HB3	5:L:282:HOH:O	2.15	0.46
1:C:78:ILE:HG22	1:C:79:THR:N	2.31	0.46
1:B:150:TYR:CE1	1:B:178:LYS:HD3	2.51	0.46
1:E:81:ASP:HA	1:E:99:GLN:O	2.16	0.46
1:K:92:ALA:HB2	1:K:117:THR:HB	1.98	0.46
1:J:212:VAL:HG21	1:J:250:ILE:HB	1.98	0.45
1:E:113:ALA:O	1:E:116:LYS:HG2	2.15	0.45
1:E:30:SER:HA	1:E:38:PHE:CE2	2.51	0.45
2:B:268:PEP:C1	3:B:269:A5P:H12	2.46	0.45
1:F:28:ARG:HG2	1:F:28:ARG:NH1	2.32	0.45
1:J:203:PHE:C	1:J:206:PRO:HD2	2.36	0.45
1:K:230:ALA:HB3	1:K:234:ALA:HA	1.98	0.45
1:D:52:ILE:HG23	1:D:53:HIS:CD2	2.51	0.45
1:H:3:LYS:N	5:H:369:HOH:O	2.48	0.45
1:F:213:ALA:HB2	1:G:213:ALA:HB2	1.98	0.45
1:F:189:LEU:HD11	1:F:200:MET:HE2	1.98	0.45
1:I:60:LEU:C	1:I:60:LEU:HD23	2.37	0.45
1:G:195:ASP:HA	1:H:136:ASN:HD21	1.82	0.45
1:H:5:LEU:HD12	1:H:37:GLU:O	2.15	0.45
1:C:30:SER:HA	1:C:38:PHE:CE2	2.52	0.45
1:F:35:GLU:N	1:F:35:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:HA	5:B:301:HOH:O	2.17	0.45
1:K:131:PRO:HG3	5:L:293:HOH:O	2.16	0.45
1:E:227:PRO:HB3	1:E:237:ALA:CB	2.44	0.45
1:K:40:PHE:O	1:K:79:THR:HG22	2.16	0.45
1:K:27:LYS:HD3	1:K:74:PHE:O	2.17	0.45
1:I:228:GLU:HG2	5:I:459:HOH:O	2.16	0.45
1:G:239:PRO:HG2	1:G:242:GLN:NE2	2.32	0.45
1:B:65:LYS:NZ	1:B:68:ARG:NH1	2.65	0.45
1:B:25:GLU:HG2	1:B:240:LEU:HD22	1.99	0.45
1:D:10:PRO:HG3	1:D:22:VAL:HG21	1.97	0.45
1:B:93:GLU:HG3	5:B:303:HOH:O	2.17	0.45
1:L:254:ARG:HD2	5:L:362:HOH:O	2.17	0.45
1:D:66:ALA:O	1:D:70:VAL:HG23	2.17	0.45
1:J:61:GLU:HG2	5:J:347:HOH:O	2.17	0.45
1:F:141:LEU:HD12	1:F:149:ILE:HG23	1.98	0.45
1:D:29:LEU:HD13	1:D:247:ILE:HD12	1.99	0.45
1:I:184:THR:CG2	1:I:222:GLU:H	2.30	0.45
1:D:96:ASP:CB	1:D:97:ILE:HD12	2.47	0.45
1:C:223:THR:OG1	1:C:240:LEU:HA	2.17	0.45
1:D:201:ARG:NH2	1:D:234:ALA:O	2.49	0.45
1:C:8:ALA:HA	1:C:221:MET:O	2.17	0.45
1:K:216:CYS:HA	5:K:325:HOH:O	2.17	0.45
1:I:30:SER:HA	1:I:38:PHE:CE2	2.52	0.44
1:K:92:ALA:CB	1:K:117:THR:HB	2.47	0.44
1:J:10:PRO:HD3	1:J:22:VAL:HG11	1.99	0.44
1:D:248:GLU:HB3	5:D:324:HOH:O	2.17	0.44
1:F:239:PRO:HG2	1:F:242:GLN:NE2	2.31	0.44
1:K:49:ARG:HD2	3:K:269:A5P:O4	2.17	0.44
1:K:60:LEU:O	1:K:64:VAL:HG23	2.18	0.44
1:K:150:TYR:HB3	1:K:180:ILE:HD13	1.98	0.44
1:D:3:LYS:HB2	1:D:35:GLU:O	2.17	0.44
1:L:258:SER:HA	1:L:261:TYR:CE2	2.51	0.44
1:I:140:LYS:HG2	1:J:52:ILE:HB	2.00	0.44
1:K:193:LEU:HD12	1:K:197:SER:O	2.17	0.44
1:D:200:MET:HB2	1:D:202:GLU:HG2	1.99	0.44
1:C:184:THR:HG21	1:C:222:GLU:H	1.82	0.44
1:H:102:ALA:HB2	1:H:154:ARG:HD3	1.97	0.44
4:D:268:1NT:O2P	4:D:268:1NT:CI3	2.66	0.44
1:H:207:LEU:HB2	5:H:276:HOH:O	2.18	0.44
2:H:268:PEP:C3	3:H:269:A5P:H12	2.48	0.44
1:H:234:ALA:N	1:H:235:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:LEU:HB2	1:E:196:LYS:O	2.17	0.44
1:G:22:VAL:O	1:G:26:ILE:HG12	2.17	0.44
1:G:147:LYS:NZ	5:G:300:HOH:O	2.47	0.44
1:E:250:ILE:HD12	1:E:251:LEU:N	2.32	0.44
1:A:232:SER:HA	5:A:335:HOH:O	2.18	0.44
1:K:82:ILE:HG13	1:K:82:ILE:O	2.17	0.44
1:L:247:ILE:HA	1:L:250:ILE:HD11	2.00	0.44
1:I:246:ILE:O	1:I:250:ILE:HG23	2.18	0.44
1:B:68:ARG:O	1:B:72:GLU:HG3	2.18	0.44
1:K:89:GLU:N	1:K:90:PRO:HD2	2.33	0.44
1:F:41:LYS:HB2	1:F:79:THR:CG2	2.47	0.44
1:L:205:PHE:HB3	1:L:206:PRO:HD3	1.99	0.44
1:F:201:ARG:NH1	1:F:237:ALA:O	2.51	0.44
1:A:156:THR:HG21	1:D:158:PHE:HZ	1.82	0.44
1:D:46:LYS:CB	1:D:49:ARG:HD3	2.48	0.44
1:K:69:LYS:HA	1:K:72:GLU:HG2	2.00	0.43
1:F:89:GLU:HB3	1:F:90:PRO:CD	2.48	0.43
1:F:11:ASN:HD22	1:F:232:SER:HB3	1.83	0.43
1:F:60:LEU:C	1:F:60:LEU:HD23	2.38	0.43
1:H:154:ARG:HH21	1:H:163:LEU:CD1	2.32	0.43
1:D:239:PRO:HB2	1:D:242:GLN:HG3	2.00	0.43
1:I:68:ARG:NH2	5:I:369:HOH:O	2.50	0.43
1:F:41:LYS:HD3	1:F:41:LYS:C	2.38	0.43
1:K:106:ARG:O	1:L:48:ASN:HA	2.18	0.43
1:L:189:LEU:HD21	1:L:200:MET:CE	2.48	0.43
1:B:3:LYS:N	5:B:381:HOH:O	2.50	0.43
1:C:4:PHE:HZ	1:C:219:VAL:HG13	1.82	0.43
1:B:151:LEU:CB	1:B:173:MET:HE1	2.28	0.43
1:J:184:THR:HG22	1:J:221:MET:HA	2.01	0.43
1:J:261:TYR:HA	1:K:209:ARG:HH12	1.83	0.43
1:K:41:LYS:HZ2	1:K:220:PHE:HZ	1.66	0.43
1:F:97:ILE:HG12	1:F:120:ALA:CB	2.48	0.43
1:L:30:SER:HA	1:L:38:PHE:CD2	2.53	0.43
1:B:88:ALA:HB3	5:B:293:HOH:O	2.17	0.43
2:E:268:PEP:O1P	2:E:268:PEP:H32	2.17	0.43
1:E:49:ARG:NE	1:E:54:SER:HB3	2.26	0.43
1:K:206:PRO:HG3	1:K:209:ARG:HH21	1.84	0.43
1:I:238:LEU:N	1:I:238:LEU:CD1	2.82	0.43
1:F:51:SER:HB2	1:F:195:ASP:HB2	2.00	0.43
1:H:201:ARG:HH21	1:H:235:PRO:C	2.22	0.43
1:I:219:VAL:HG12	1:I:221:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ILE:CG2	1:F:79:THR:N	2.82	0.43
1:F:227:PRO:HB3	1:F:237:ALA:HB3	2.00	0.43
1:L:154:ARG:NH2	1:L:188:GLN:NE2	2.56	0.43
1:K:238:LEU:HD21	1:K:246:ILE:CD1	2.48	0.43
3:F:269:A5P:O4	3:F:269:A5P:C1	2.66	0.43
1:L:100:ILE:HD12	1:L:100:ILE:N	2.33	0.43
1:C:46:LYS:HD3	5:C:323:HOH:O	2.18	0.43
1:G:185:HIS:O	1:G:188:GLN:HG2	2.19	0.43
1:A:170:LEU:CB	1:A:171:PRO:HD3	2.49	0.43
1:B:78:ILE:CG2	1:B:79:THR:N	2.82	0.43
1:D:5:LEU:HD13	1:D:6:VAL:N	2.33	0.43
1:C:4:PHE:CE1	1:C:218:GLY:HA2	2.54	0.43
1:E:13:ILE:HD12	1:E:44:PHE:HA	2.00	0.43
1:G:252:GLU:O	1:G:255:GLU:HB3	2.18	0.43
1:F:30:SER:HA	1:F:38:PHE:CD2	2.53	0.43
1:H:237:ALA:CB	5:H:274:HOH:O	2.65	0.43
1:F:252:GLU:O	1:F:255:GLU:HB3	2.18	0.43
1:H:87:GLN:O	1:H:90:PRO:HG2	2.19	0.43
1:D:62:TYR:O	1:D:65:LYS:HB3	2.19	0.43
1:A:258:SER:HA	1:A:261:TYR:CE2	2.54	0.43
1:H:122:ASN:HA	1:H:150:TYR:HB2	2.00	0.43
1:D:36:VAL:HB	1:D:38:PHE:CE2	2.54	0.43
1:F:141:LEU:CD1	1:F:149:ILE:HG23	2.48	0.42
1:J:228:GLU:HG2	1:J:229:LYS:N	2.34	0.42
1:B:30:SER:HA	1:B:38:PHE:CE2	2.54	0.42
1:D:255:GLU:HB3	5:D:304:HOH:O	2.19	0.42
1:K:41:LYS:HA	1:K:79:THR:O	2.19	0.42
1:L:78:ILE:HG22	1:L:79:THR:N	2.33	0.42
1:G:89:GLU:HB3	1:G:90:PRO:CD	2.49	0.42
1:C:49:ARG:HD2	3:C:269:A5P:C5	2.49	0.42
1:C:136:ASN:ND2	1:D:195:ASP:HA	2.33	0.42
1:L:99:GLN:C	1:L:100:ILE:HD12	2.40	0.42
1:G:247:ILE:O	1:G:250:ILE:HG13	2.19	0.42
1:D:41:LYS:HE2	1:D:220:PHE:HZ	1.84	0.42
1:D:64:VAL:HG13	1:D:94:VAL:HG12	2.01	0.42
1:B:11:ASN:HD21	1:B:46:LYS:CE	2.31	0.42
1:K:99:GLN:NE2	1:K:124:LYS:HE2	2.34	0.42
1:I:41:LYS:C	1:I:41:LYS:HD3	2.40	0.42
1:D:78:ILE:HG22	1:D:79:THR:N	2.34	0.42
1:F:256:VAL:HG22	5:F:315:HOH:O	2.18	0.42
1:A:189:LEU:HD21	1:A:200:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ASN:ND2	5:G:387:HOH:O	2.51	0.42
2:K:268:PEP:H32	2:K:268:PEP:O1P	2.15	0.42
1:F:195:ASP:OD1	1:F:196:LYS:HG3	2.19	0.42
1:J:247:ILE:O	1:J:250:ILE:HG13	2.20	0.42
1:J:25:GLU:HA	1:J:28:ARG:HH11	1.85	0.42
3:A:269:A5P:HC4	3:A:269:A5P:H12	1.81	0.42
1:D:106:ARG:HA	5:D:297:HOH:O	2.18	0.42
1:J:256:VAL:O	1:J:256:VAL:HG12	2.19	0.42
1:B:99:GLN:NE2	1:B:124:LYS:HE3	2.34	0.42
1:I:154:ARG:HH21	1:I:163:LEU:CD1	2.32	0.42
1:F:243:LEU:HD12	1:F:247:ILE:HD11	2.01	0.42
1:J:22:VAL:O	1:J:26:ILE:HG12	2.19	0.42
1:L:212:VAL:HG23	1:L:253:ILE:HG21	2.01	0.42
1:F:84:GLU:HG3	5:F:307:HOH:O	2.20	0.42
1:C:16:GLU:O	1:C:20:LEU:HG	2.19	0.42
1:H:89:GLU:HB3	1:H:90:PRO:CD	2.49	0.42
1:L:193:LEU:HB2	1:L:196:LYS:HG3	2.02	0.42
1:D:87:GLN:O	1:D:91:VAL:HB	2.19	0.42
1:J:111:LEU:HD22	1:J:141:LEU:HD21	2.02	0.42
1:G:154:ARG:HH21	1:G:163:LEU:CD1	2.33	0.42
1:F:19:LEU:HD12	1:F:66:ALA:HB1	2.02	0.42
1:D:5:LEU:HD12	1:D:7:ILE:HG13	2.02	0.42
1:L:176:TRP:O	1:L:177:ALA:HB2	2.20	0.42
1:H:154:ARG:CD	2:H:268:PEP:O3P	2.66	0.42
1:J:234:ALA:N	1:J:235:PRO:CD	2.82	0.42
1:B:263:THR:HG22	1:B:264:ILE:N	2.35	0.42
1:L:246:ILE:O	1:L:250:ILE:HG12	2.19	0.42
1:D:46:LYS:HB3	1:D:49:ARG:HD3	2.01	0.42
1:E:210:ALA:HB2	1:H:214:VAL:HG23	2.02	0.42
1:G:201:ARG:HD3	1:G:204:ILE:HD12	2.01	0.41
1:E:60:LEU:O	1:E:60:LEU:HD23	2.20	0.41
1:F:187:VAL:HG21	1:F:204:ILE:HG12	2.02	0.41
1:K:86:TRP:HD1	5:K:302:HOH:O	2.02	0.41
1:J:254:ARG:O	1:J:258:SER:HB3	2.21	0.41
1:J:201:ARG:HB2	1:J:201:ARG:CZ	2.50	0.41
1:C:140:LYS:HG2	1:D:52:ILE:HB	2.02	0.41
1:C:4:PHE:CZ	1:C:219:VAL:HG13	2.55	0.41
1:H:78:ILE:HG22	1:H:79:THR:N	2.35	0.41
2:H:268:PEP:H32	2:H:268:PEP:O1P	2.16	0.41
1:A:12:ALA:HB2	1:A:46:LYS:HD3	2.03	0.41
1:L:14:GLU:HB2	1:L:18:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:GLN:NE2	1:D:104:LEU:HD11	2.35	0.41
1:C:128:PHE:HB3	5:D:272:HOH:O	2.19	0.41
1:G:5:LEU:HD12	1:G:37:GLU:HB3	2.02	0.41
1:E:10:PRO:HG3	1:E:22:VAL:HG21	2.02	0.41
1:H:184:THR:CG2	1:H:221:MET:HA	2.47	0.41
1:B:201:ARG:HA	1:B:204:ILE:HG13	2.02	0.41
1:L:87:GLN:O	1:L:90:PRO:HG2	2.20	0.41
1:I:222:GLU:O	1:I:238:LEU:HD13	2.21	0.41
1:K:13:ILE:HD11	1:K:67:LEU:HD11	2.03	0.41
1:C:47:ALA:HB3	1:C:83:HIS:CD2	2.54	0.41
1:I:4:PHE:CE2	1:I:219:VAL:HG23	2.55	0.41
1:J:52:ILE:O	1:J:52:ILE:HG13	2.19	0.41
1:K:169:SER:O	1:K:173:MET:HG3	2.21	0.41
1:F:14:GLU:OE1	1:F:231:LEU:HG	2.20	0.41
1:F:60:LEU:O	1:F:64:VAL:HG23	2.21	0.41
1:D:55:PHE:CZ	1:D:57:GLY:HA2	2.55	0.41
1:A:132:TRP:HA	1:A:176:TRP:CH2	2.56	0.41
1:E:71:LYS:HE3	5:E:339:HOH:O	2.20	0.41
1:K:264:ILE:HG13	1:K:264:ILE:H	1.74	0.41
1:J:5:LEU:HD12	1:J:37:GLU:O	2.20	0.41
1:C:3:LYS:HD2	1:C:35:GLU:O	2.21	0.41
1:J:189:LEU:HD21	1:J:200:MET:HE1	2.03	0.41
1:J:3:LYS:N	5:J:453:HOH:O	2.54	0.41
1:K:201:ARG:NH1	1:K:237:ALA:O	2.52	0.41
1:K:19:LEU:H	1:K:19:LEU:CD1	2.34	0.41
1:E:5:LEU:HD22	1:E:7:ILE:HG13	2.03	0.41
1:E:116:LYS:HG3	1:E:117:THR:N	2.35	0.41
1:L:201:ARG:NH2	1:L:234:ALA:O	2.54	0.41
1:L:187:VAL:HG21	1:L:204:ILE:HG12	2.03	0.41
1:K:67:LEU:HD21	1:K:80:THR:HB	2.03	0.41
1:L:14:GLU:CD	1:L:231:LEU:HG	2.41	0.41
1:K:207:LEU:HB2	5:K:278:HOH:O	2.20	0.41
1:E:180:ILE:HG22	1:E:181:TYR:N	2.36	0.41
1:D:161:ASN:HA	1:D:190:PRO:HG2	2.03	0.41
1:E:219:VAL:HG12	1:E:221:MET:HG3	2.03	0.41
1:H:226:GLU:HA	1:H:227:PRO:HD2	1.90	0.41
1:K:50:SER:O	1:L:136:ASN:HB3	2.21	0.41
1:L:89:GLU:N	1:L:90:PRO:HD2	2.36	0.41
1:D:60:LEU:C	1:D:60:LEU:HD23	2.42	0.41
1:F:13:ILE:HD12	1:F:44:PHE:HA	2.03	0.41
1:G:89:GLU:HG3	5:G:404:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:237:ALA:HB2	5:I:403:HOH:O	2.21	0.41
1:K:96:ASP:HB3	5:K:311:HOH:O	2.21	0.41
2:C:268:PEP:O1P	2:C:268:PEP:H32	2.21	0.40
1:F:89:GLU:HB3	1:F:90:PRO:HD3	2.03	0.40
1:F:89:GLU:N	1:F:90:PRO:HD2	2.36	0.40
1:C:97:ILE:HG12	1:C:120:ALA:HB3	2.02	0.40
1:D:11:ASN:HD22	1:D:232:SER:HB3	1.85	0.40
1:C:34:LYS:HG2	5:C:353:HOH:O	2.19	0.40
1:C:5:LEU:HD12	1:C:37:GLU:O	2.21	0.40
1:J:184:THR:CG2	1:J:221:MET:HA	2.51	0.40
1:I:44:PHE:CD1	1:I:60:LEU:HA	2.56	0.40
1:C:13:ILE:HG13	1:C:43:SER:O	2.21	0.40
1:E:52:ILE:HG23	1:E:53:HIS:HD2	1.82	0.40
1:K:11:ASN:HD21	1:K:46:LYS:CE	2.35	0.40
1:L:234:ALA:N	1:L:235:PRO:CD	2.84	0.40
1:L:193:LEU:HB2	1:L:196:LYS:O	2.21	0.40
1:K:95:ALA:O	1:K:119:ARG:HD2	2.21	0.40
1:I:165:VAL:CG2	1:I:186:SER:HB3	2.51	0.40
1:J:41:LYS:HE3	1:J:42:SER:HA	2.04	0.40
1:L:154:ARG:NH2	1:L:188:GLN:HE21	2.17	0.40
4:D:268:1NT:C1	4:D:268:1NT:HOA1	2.35	0.40
1:I:201:ARG:NH1	5:I:450:HOH:O	2.55	0.40
1:K:70:VAL:HA	5:K:316:HOH:O	2.21	0.40
1:J:83:HIS:HE1	5:J:270:HOH:O	2.03	0.40
1:I:89:GLU:HB3	1:I:90:PRO:CD	2.51	0.40
1:F:210:ALA:O	1:F:214:VAL:HG23	2.21	0.40
1:H:189:LEU:HD11	1:H:200:MET:HE2	2.02	0.40
1:F:91:VAL:O	1:F:93:GLU:N	2.55	0.40
1:F:227:PRO:CB	1:F:237:ALA:HB3	2.51	0.40
1:L:242:GLN:O	1:L:246:ILE:HG12	2.22	0.40
1:H:25:GLU:O	1:H:29:LEU:HG	2.22	0.40
1:C:52:ILE:O	1:C:52:ILE:HG13	2.21	0.40
1:F:5:LEU:N	1:F:5:LEU:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	260/267 (97%)	253 (97%)	7 (3%)	0	100	100
1	B	260/267 (97%)	253 (97%)	7 (3%)	0	100	100
1	C	260/267 (97%)	245 (94%)	15 (6%)	0	100	100
1	D	260/267 (97%)	246 (95%)	14 (5%)	0	100	100
1	E	260/267 (97%)	241 (93%)	15 (6%)	4 (2%)	13	7
1	F	260/267 (97%)	235 (90%)	22 (8%)	3 (1%)	16	10
1	G	260/267 (97%)	253 (97%)	7 (3%)	0	100	100
1	H	260/267 (97%)	251 (96%)	9 (4%)	0	100	100
1	I	260/267 (97%)	252 (97%)	8 (3%)	0	100	100
1	J	260/267 (97%)	249 (96%)	10 (4%)	1 (0%)	39	37
1	K	260/267 (97%)	237 (91%)	22 (8%)	1 (0%)	39	37
1	L	260/267 (97%)	246 (95%)	14 (5%)	0	100	100
All	All	3120/3204 (97%)	2961 (95%)	150 (5%)	9 (0%)	46	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	86	TRP
1	E	92	ALA
1	F	92	ALA
1	K	94	VAL
1	F	105	CYS
1	F	262	GLU
1	E	85	SER
1	E	190	PRO
1	J	235	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	218/223 (98%)	217 (100%)	1 (0%)	92	95
1	B	218/223 (98%)	214 (98%)	4 (2%)	66	72
1	C	218/223 (98%)	214 (98%)	4 (2%)	66	72
1	D	218/223 (98%)	213 (98%)	5 (2%)	58	62
1	E	218/223 (98%)	214 (98%)	4 (2%)	66	72
1	F	218/223 (98%)	212 (97%)	6 (3%)	51	55
1	G	218/223 (98%)	216 (99%)	2 (1%)	84	89
1	H	218/223 (98%)	217 (100%)	1 (0%)	92	95
1	I	218/223 (98%)	217 (100%)	1 (0%)	92	95
1	J	218/223 (98%)	217 (100%)	1 (0%)	92	95
1	K	218/223 (98%)	214 (98%)	4 (2%)	66	72
1	L	218/223 (98%)	216 (99%)	2 (1%)	84	89
All	All	2616/2676 (98%)	2581 (99%)	35 (1%)	76	82

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	B	65	LYS
1	B	184	THR
1	B	228	GLU
1	B	259	LYS
1	C	154	ARG
1	C	176	TRP
1	C	195	ASP
1	C	250	ILE
1	D	5	LEU
1	D	154	ARG
1	D	176	TRP
1	D	200	MET
1	D	201	ARG

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Mol	Chain	Res	Type
1	E	35	GLU
1	E	116	LYS
1	E	119	ARG
1	E	250	ILE
1	F	35	GLU
1	F	69	LYS
1	F	154	ARG
1	F	176	TRP
1	F	208	ILE
1	F	243	LEU
1	G	228	GLU
1	G	250	ILE
1	H	106	ARG
1	I	35	GLU
1	J	184	THR
1	K	3	LYS
1	K	41	LYS
1	K	154	ARG
1	K	176	TRP
1	L	69	LYS
1	L	176	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	83	HIS
1	A	136	ASN
1	A	242	GLN
1	B	11	ASN
1	B	83	HIS
1	B	99	GLN
1	B	136	ASN
1	B	175	GLN
1	B	188	GLN
1	C	11	ASN
1	C	83	HIS
1	C	136	ASN
1	C	175	GLN
1	C	242	GLN
1	D	11	ASN
1	D	53	HIS

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Mol	Chain	Res	Type
1	D	83	HIS
1	D	188	GLN
1	E	53	HIS
1	E	136	ASN
1	E	161	ASN
1	E	175	GLN
1	E	242	GLN
1	F	11	ASN
1	F	83	HIS
1	F	185	HIS
1	F	188	GLN
1	F	242	GLN
1	G	83	HIS
1	G	136	ASN
1	G	188	GLN
1	G	242	GLN
1	H	11	ASN
1	H	53	HIS
1	H	83	HIS
1	H	136	ASN
1	H	175	GLN
1	H	188	GLN
1	I	11	ASN
1	I	53	HIS
1	I	83	HIS
1	I	175	GLN
1	I	188	GLN
1	I	242	GLN
1	J	11	ASN
1	J	83	HIS
1	J	136	ASN
1	J	242	GLN
1	K	11	ASN
1	K	53	HIS
1	K	83	HIS
1	K	136	ASN
1	K	161	ASN
1	L	11	ASN
1	L	83	HIS
1	L	136	ASN
1	L	175	GLN
1	L	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

23 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	PEP	A	268	-	5,9,9	1.97	1 (20%)	8,13,13	1.44	1 (12%)
3	A5P	A	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.52	2 (14%)
2	PEP	B	268	-	5,9,9	2.00	1 (20%)	8,13,13	1.57	1 (12%)
3	A5P	B	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.50	1 (7%)
2	PEP	C	268	-	5,9,9	1.96	1 (20%)	8,13,13	1.71	1 (12%)
3	A5P	C	269	-	13,13,13	1.70	2 (15%)	14,18,18	1.53	2 (14%)
4	1NT	D	268	-	19,24,24	1.39	2 (10%)	19,37,37	0.88	1 (5%)
2	PEP	E	268	-	5,9,9	1.96	1 (20%)	8,13,13	1.79	1 (12%)
3	A5P	E	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.52	2 (14%)
2	PEP	F	268	-	5,9,9	1.96	1 (20%)	8,13,13	1.78	1 (12%)
3	A5P	F	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.49	2 (14%)
2	PEP	G	268	-	5,9,9	1.96	1 (20%)	8,13,13	1.67	1 (12%)
3	A5P	G	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.52	2 (14%)
2	PEP	H	268	-	5,9,9	1.95	1 (20%)	8,13,13	1.67	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A5P	H	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.45	1 (7%)
2	PEP	I	268	-	5,9,9	2.00	1 (20%)	8,13,13	1.57	1 (12%)
3	A5P	I	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.55	2 (14%)
2	PEP	J	268	-	5,9,9	1.98	1 (20%)	8,13,13	1.53	1 (12%)
3	A5P	J	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.50	1 (7%)
2	PEP	K	268	-	5,9,9	1.97	1 (20%)	8,13,13	1.87	1 (12%)
3	A5P	K	269	-	13,13,13	1.69	2 (15%)	14,18,18	1.51	2 (14%)
2	PEP	L	268	-	5,9,9	1.97	1 (20%)	8,13,13	1.78	1 (12%)
3	A5P	L	269	-	13,13,13	1.70	2 (15%)	14,18,18	1.50	2 (14%)

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
2	PEP	A	268	-	-	0/5/9/9	0/0/0/0
3	A5P	A	269	-	-	0/16/16/16	0/0/0/0
2	PEP	B	268	-	-	0/5/9/9	0/0/0/0
3	A5P	B	269	-	-	0/16/16/16	0/0/0/0
2	PEP	C	268	-	-	0/5/9/9	0/0/0/0
3	A5P	C	269	-	-	0/16/16/16	0/0/0/0
4	1NT	D	268	-	-	0/25/35/35	0/0/0/0
2	PEP	E	268	-	-	0/5/9/9	0/0/0/0
3	A5P	E	269	-	-	0/16/16/16	0/0/0/0
2	PEP	F	268	-	-	0/5/9/9	0/0/0/0
3	A5P	F	269	-	-	0/16/16/16	0/0/0/0
2	PEP	G	268	-	-	0/5/9/9	0/0/0/0
3	A5P	G	269	-	-	0/16/16/16	0/0/0/0
2	PEP	H	268	-	-	0/5/9/9	0/0/0/0
3	A5P	H	269	-	-	0/16/16/16	0/0/0/0
2	PEP	I	268	-	-	0/5/9/9	0/0/0/0
3	A5P	I	269	-	-	0/16/16/16	0/0/0/0
2	PEP	J	268	-	-	0/5/9/9	0/0/0/0
3	A5P	J	269	-	-	0/16/16/16	0/0/0/0
2	PEP	K	268	-	-	0/5/9/9	0/0/0/0
3	A5P	K	269	-	-	0/16/16/16	0/0/0/0
2	PEP	L	268	-	-	0/5/9/9	0/0/0/0
3	A5P	L	269	-	-	0/16/16/16	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	269	A5P	O1-C1	-4.40	1.23	1.42
3	I	269	A5P	O1-C1	-4.40	1.23	1.42
3	C	269	A5P	O1-C1	-4.39	1.23	1.42
3	F	269	A5P	O1-C1	-4.39	1.23	1.42
3	J	269	A5P	O1-C1	-4.39	1.23	1.42
3	E	269	A5P	O1-C1	-4.38	1.23	1.42
3	B	269	A5P	O1-C1	-4.37	1.23	1.42
3	K	269	A5P	O1-C1	-4.37	1.23	1.42
3	A	269	A5P	O1-C1	-4.37	1.23	1.42
3	G	269	A5P	O1-C1	-4.37	1.23	1.42
3	H	269	A5P	O1-C1	-4.37	1.23	1.42
3	I	269	A5P	P-O1P	3.09	1.61	1.51
3	A	269	A5P	P-O1P	3.10	1.61	1.51
3	K	269	A5P	P-O1P	3.11	1.61	1.51
3	J	269	A5P	P-O1P	3.11	1.61	1.51
3	L	269	A5P	P-O1P	3.11	1.61	1.51
3	F	269	A5P	P-O1P	3.12	1.61	1.51
3	E	269	A5P	P-O1P	3.12	1.61	1.51
3	B	269	A5P	P-O1P	3.12	1.61	1.51
3	G	269	A5P	P-O1P	3.12	1.61	1.51
4	D	268	1NT	P-O3P	3.12	1.61	1.51
3	H	269	A5P	P-O1P	3.12	1.61	1.51
3	C	269	A5P	P-O1P	3.13	1.61	1.51
2	F	268	PEP	C3-C2	3.25	1.39	1.33
2	E	268	PEP	C3-C2	3.28	1.39	1.33
2	H	268	PEP	C3-C2	3.28	1.39	1.33
4	D	268	1NT	O3-C2	3.28	1.43	1.40
2	G	268	PEP	C3-C2	3.30	1.39	1.33
2	A	268	PEP	C3-C2	3.30	1.39	1.33
2	C	268	PEP	C3-C2	3.30	1.39	1.33
2	K	268	PEP	C3-C2	3.32	1.39	1.33
2	L	268	PEP	C3-C2	3.32	1.39	1.33
2	J	268	PEP	C3-C2	3.33	1.39	1.33
2	I	268	PEP	C3-C2	3.35	1.39	1.33
2	B	268	PEP	C3-C2	3.38	1.39	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	268	PEP	P-O2-C2	-4.76	112.38	122.96
2	E	268	PEP	P-O2-C2	-4.54	112.86	122.96
2	F	268	PEP	P-O2-C2	-4.53	112.90	122.96
2	L	268	PEP	P-O2-C2	-4.50	112.97	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	268	PEP	P-O2-C2	-4.33	113.33	122.96
2	H	268	PEP	P-O2-C2	-4.17	113.69	122.96
2	G	268	PEP	P-O2-C2	-4.13	113.78	122.96
2	I	268	PEP	P-O2-C2	-3.96	114.16	122.96
2	B	268	PEP	P-O2-C2	-3.91	114.27	122.96
2	J	268	PEP	P-O2-C2	-3.72	114.69	122.96
2	A	268	PEP	P-O2-C2	-3.41	115.37	122.96
4	D	268	1NT	OP4-PA-OP2	2.12	112.54	107.14
3	A	269	A5P	O3P-P-O5	2.22	112.96	106.56
3	G	269	A5P	O3P-P-O5	2.22	112.96	106.56
3	E	269	A5P	O3P-P-O5	2.34	113.30	106.56
3	L	269	A5P	O3P-P-O5	2.36	113.37	106.56
3	K	269	A5P	O3P-P-O5	2.43	113.56	106.56
3	F	269	A5P	O3P-P-O5	2.47	113.66	106.56
3	C	269	A5P	O3P-P-O5	2.47	113.68	106.56
3	I	269	A5P	O3P-P-O5	2.65	114.18	106.56
3	I	269	A5P	O1-C1-C2	4.26	120.36	111.10
3	J	269	A5P	O1-C1-C2	4.31	120.46	111.10
3	H	269	A5P	O1-C1-C2	4.39	120.65	111.10
3	F	269	A5P	O1-C1-C2	4.40	120.66	111.10
3	C	269	A5P	O1-C1-C2	4.45	120.77	111.10
3	B	269	A5P	O1-C1-C2	4.45	120.78	111.10
3	K	269	A5P	O1-C1-C2	4.49	120.87	111.10
3	L	269	A5P	O1-C1-C2	4.51	120.89	111.10
3	G	269	A5P	O1-C1-C2	4.58	121.07	111.10
3	E	269	A5P	O1-C1-C2	4.60	121.11	111.10
3	A	269	A5P	O1-C1-C2	4.67	121.24	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	268	PEP	2	0
3	A	269	A5P	2	0
2	B	268	PEP	4	0
3	B	269	A5P	6	0
2	C	268	PEP	2	0
3	C	269	A5P	3	0
4	D	268	1NT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	268	PEP	1	0
2	F	268	PEP	2	0
3	F	269	A5P	4	0
2	G	268	PEP	1	0
3	G	269	A5P	3	0
2	H	268	PEP	5	0
3	H	269	A5P	3	0
2	I	268	PEP	5	0
3	I	269	A5P	3	0
2	J	268	PEP	3	0
3	J	269	A5P	2	0
2	K	268	PEP	2	0
3	K	269	A5P	1	0
2	L	268	PEP	2	0
3	L	269	A5P	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	262/267 (98%)	0.29	12 (4%) 36 45	16, 27, 50, 74	0
1	B	262/267 (98%)	0.40	19 (7%) 18 24	16, 28, 49, 71	0
1	C	262/267 (98%)	0.87	32 (12%) 5 7	23, 47, 65, 72	0
1	D	262/267 (98%)	1.29	58 (22%) 1 1	24, 52, 72, 79	0
1	E	262/267 (98%)	1.39	71 (27%) 1 1	26, 58, 82, 90	0
1	F	262/267 (98%)	1.74	81 (30%) 1 1	30, 60, 78, 89	0
1	G	262/267 (98%)	0.47	15 (5%) 27 35	19, 32, 61, 86	0
1	H	262/267 (98%)	0.46	17 (6%) 22 29	19, 31, 56, 75	0
1	I	262/267 (98%)	0.40	17 (6%) 22 29	19, 29, 48, 69	0
1	J	262/267 (98%)	0.48	19 (7%) 18 24	19, 30, 59, 79	0
1	K	262/267 (98%)	1.74	96 (36%) 0 0	30, 62, 82, 87	0
1	L	262/267 (98%)	1.23	54 (20%) 1 1	26, 50, 68, 86	0
All	All	3144/3204 (98%)	0.90	491 (15%) 3 4	16, 40, 74, 90	0

All (491) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	264	ILE	11.4
1	L	193	LEU	9.7
1	F	193	LEU	8.4
1	H	264	ILE	8.3
1	E	195	ASP	8.0
1	K	63	GLY	7.8
1	F	264	ILE	7.8
1	L	195	ASP	7.7
1	G	263	THR	7.6
1	F	196	LYS	7.3
1	L	264	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
1	F	194	GLY	7.2
1	F	94	VAL	7.1
1	F	263	THR	7.0
1	J	263	THR	6.9
1	J	264	ILE	6.9
1	H	193	LEU	6.8
1	D	264	ILE	6.8
1	D	196	LYS	6.7
1	K	195	ASP	6.6
1	F	195	ASP	6.6
1	K	67	LEU	6.3
1	F	220	PHE	6.2
1	L	196	LYS	6.1
1	L	197	SER	6.0
1	K	74	PHE	5.8
1	D	195	ASP	5.8
1	K	192	GLY	5.8
1	L	194	GLY	5.7
1	F	192	GLY	5.7
1	C	194	GLY	5.7
1	E	193	LEU	5.7
1	I	193	LEU	5.7
1	E	231	LEU	5.7
1	F	198	GLY	5.7
1	K	196	LYS	5.6
1	H	263	THR	5.5
1	L	235	PRO	5.5
1	J	193	LEU	5.5
1	E	147	LYS	5.4
1	I	263	THR	5.4
1	L	198	GLY	5.4
1	C	193	LEU	5.4
1	F	199	GLY	5.4
1	A	263	THR	5.3
1	H	192	GLY	5.3
1	G	194	GLY	5.2
1	H	194	GLY	5.2
1	B	264	ILE	5.2
1	C	235	PRO	5.2
1	H	235	PRO	5.1
1	K	193	LEU	5.1
1	F	57	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	72	GLU	5.0
1	E	16	GLU	5.0
1	D	220	PHE	5.0
1	D	263	THR	5.0
1	A	264	ILE	4.9
1	K	198	GLY	4.9
1	K	72	GLU	4.9
1	E	196	LYS	4.9
1	C	264	ILE	4.9
1	E	198	GLY	4.8
1	F	7	ILE	4.8
1	D	70	VAL	4.8
1	D	16	GLU	4.8
1	E	220	PHE	4.7
1	J	194	GLY	4.7
1	B	263	THR	4.7
1	L	191	GLY	4.7
1	F	74	PHE	4.7
1	L	95	ALA	4.7
1	F	235	PRO	4.6
1	K	7	ILE	4.6
1	K	264	ILE	4.6
1	E	61	GLU	4.6
1	F	70	VAL	4.5
1	L	113	ALA	4.5
1	H	195	ASP	4.5
1	K	116	LYS	4.4
1	K	118	GLY	4.4
1	K	20	LEU	4.4
1	K	220	PHE	4.4
1	F	141	LEU	4.3
1	C	20	LEU	4.3
1	K	86	TRP	4.3
1	D	197	SER	4.2
1	F	197	SER	4.2
1	E	7	ILE	4.1
1	D	20	LEU	4.1
1	E	219	VAL	4.1
1	I	264	ILE	4.1
1	F	144	GLY	4.1
1	E	146	ALA	4.1
1	F	176	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	145	GLY	4.1
1	E	17	GLU	4.1
1	A	195	ASP	4.1
1	L	220	PHE	4.1
1	B	194	GLY	4.1
1	K	34	LYS	4.1
1	L	54	SER	4.1
1	K	200	MET	4.1
1	B	192	GLY	4.1
1	B	195	ASP	4.0
1	K	197	SER	4.0
1	K	241	SER	4.0
1	E	65	LYS	4.0
1	F	72	GLU	3.9
1	F	228	GLU	3.9
1	G	192	GLY	3.9
1	K	57	GLY	3.9
1	E	20	LEU	3.9
1	D	69	LYS	3.9
1	B	193	LEU	3.9
1	J	198	GLY	3.9
1	F	221	MET	3.9
1	D	7	ILE	3.8
1	D	235	PRO	3.8
1	K	8	ALA	3.8
1	K	16	GLU	3.8
1	K	142	LYS	3.8
1	K	219	VAL	3.8
1	F	6	VAL	3.7
1	D	93	GLU	3.7
1	L	123	VAL	3.7
1	E	143	PHE	3.7
1	I	235	PRO	3.7
1	J	192	GLY	3.7
1	E	52	ILE	3.7
1	C	195	ASP	3.7
1	D	193	LEU	3.7
1	L	94	VAL	3.6
1	I	192	GLY	3.6
1	K	221	MET	3.6
1	H	197	SER	3.6
1	C	143	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	6	VAL	3.6
1	F	68	ARG	3.6
1	F	89	GLU	3.6
1	K	17	GLU	3.6
1	A	193	LEU	3.6
1	K	73	GLU	3.6
1	E	194	GLY	3.5
1	J	220	PHE	3.5
1	E	22	VAL	3.5
1	F	249	ALA	3.5
1	K	263	THR	3.5
1	E	69	LYS	3.5
1	F	219	VAL	3.5
1	L	111	LEU	3.5
1	F	262	GLU	3.4
1	F	150	TYR	3.4
1	F	115	ALA	3.4
1	C	220	PHE	3.4
1	K	6	VAL	3.4
1	K	69	LYS	3.4
1	J	195	ASP	3.4
1	C	93	GLU	3.4
1	D	74	PHE	3.4
1	K	70	VAL	3.4
1	K	138	VAL	3.4
1	B	235	PRO	3.4
1	F	111	LEU	3.3
1	K	76	LEU	3.3
1	K	61	GLU	3.3
1	K	93	GLU	3.3
1	K	89	GLU	3.3
1	L	190	PRO	3.3
1	F	76	LEU	3.3
1	L	100	ILE	3.3
1	J	260	TYR	3.3
1	K	191	GLY	3.3
1	E	142	LYS	3.3
1	F	18	LEU	3.3
1	B	197	SER	3.3
1	L	70	VAL	3.3
1	H	196	LYS	3.2
1	C	70	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	142	LYS	3.2
1	L	192	GLY	3.2
1	K	117	THR	3.2
1	K	60	LEU	3.2
1	L	93	GLU	3.2
1	K	26	ILE	3.2
1	B	220	PHE	3.2
1	F	143	PHE	3.2
1	F	93	GLU	3.2
1	I	194	GLY	3.1
1	K	91	VAL	3.1
1	G	193	LEU	3.1
1	K	143	PHE	3.1
1	H	198	GLY	3.1
1	F	181	TYR	3.1
1	E	227	PRO	3.1
1	D	200	MET	3.1
1	E	35	GLU	3.1
1	F	189	LEU	3.1
1	L	143	PHE	3.1
1	D	100	ILE	3.1
1	D	194	GLY	3.1
1	K	65	LYS	3.1
1	F	147	LYS	3.0
1	E	180	ILE	3.0
1	K	194	GLY	3.0
1	G	220	PHE	3.0
1	E	115	ALA	3.0
1	K	232	SER	3.0
1	C	147	LYS	3.0
1	F	20	LEU	3.0
1	F	16	GLU	3.0
1	L	144	GLY	3.0
1	D	35	GLU	3.0
1	E	114	ALA	3.0
1	K	183	ALA	3.0
1	E	75	GLY	2.9
1	J	190	PRO	2.9
1	L	89	GLU	2.9
1	F	100	ILE	2.9
1	F	132	TRP	2.9
1	K	111	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	226	GLU	2.9
1	D	198	GLY	2.9
1	L	18	LEU	2.9
1	K	152	THR	2.9
1	J	228	GLU	2.9
1	G	195	ASP	2.9
1	K	95	ALA	2.8
1	E	86	TRP	2.8
1	D	183	ALA	2.8
1	K	231	LEU	2.8
1	E	118	GLY	2.8
1	F	35	GLU	2.8
1	C	86	TRP	2.8
1	K	55	PHE	2.8
1	L	90	PRO	2.8
1	C	183	ALA	2.8
1	K	35	GLU	2.8
1	C	192	GLY	2.8
1	D	94	VAL	2.8
1	F	55	PHE	2.8
1	D	57	GLY	2.8
1	B	219	VAL	2.8
1	F	61	GLU	2.8
1	F	62	TYR	2.8
1	K	181	TYR	2.8
1	K	178	LYS	2.8
1	E	57	GLY	2.8
1	E	102	ALA	2.8
1	K	75	GLY	2.8
1	D	184	THR	2.8
1	D	89	GLU	2.8
1	K	228	GLU	2.8
1	L	17	GLU	2.8
1	F	67	LEU	2.8
1	K	52	ILE	2.8
1	E	55	PHE	2.7
1	C	51	SER	2.7
1	C	145	GLY	2.7
1	L	147	LYS	2.7
1	K	115	ALA	2.7
1	J	196	LYS	2.7
1	K	235	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	2.7
1	E	76	LEU	2.7
1	F	251	LEU	2.7
1	K	180	ILE	2.7
1	D	68	ARG	2.7
1	F	79	THR	2.7
1	F	184	THR	2.7
1	G	259	LYS	2.7
1	D	228	GLU	2.7
1	E	197	SER	2.7
1	J	235	PRO	2.7
1	E	221	MET	2.7
1	D	18	LEU	2.6
1	F	152	THR	2.6
1	F	191	GLY	2.6
1	H	220	PHE	2.6
1	F	3	LYS	2.6
1	L	65	LYS	2.6
1	K	190	PRO	2.6
1	F	182	ASP	2.6
1	K	103	PHE	2.6
1	K	18	LEU	2.6
1	E	264	ILE	2.6
1	F	248	GLU	2.6
1	K	23	GLY	2.6
1	A	220	PHE	2.6
1	D	238	LEU	2.6
1	L	263	THR	2.6
1	B	198	GLY	2.6
1	D	145	GLY	2.6
1	D	256	VAL	2.6
1	K	27	LYS	2.6
1	E	40	PHE	2.6
1	D	176	TRP	2.6
1	C	19	LEU	2.6
1	E	70	VAL	2.6
1	K	64	VAL	2.6
1	C	54	SER	2.5
1	K	41	LYS	2.5
1	H	184	THR	2.5
1	D	95	ALA	2.5
1	L	200	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	219	VAL	2.5
1	C	196	LYS	2.5
1	E	62	TYR	2.5
1	L	103	PHE	2.5
1	B	200	MET	2.5
1	E	218	GLY	2.5
1	F	4	PHE	2.5
1	K	226	GLU	2.5
1	L	114	ALA	2.5
1	L	132	TRP	2.5
1	F	54	SER	2.5
1	D	63	GLY	2.5
1	A	184	THR	2.5
1	F	146	ALA	2.5
1	L	146	ALA	2.5
1	D	143	PHE	2.5
1	L	231	LEU	2.5
1	B	7	ILE	2.5
1	F	36	VAL	2.5
1	F	187	VAL	2.5
1	I	180	ILE	2.5
1	K	22	VAL	2.5
1	F	200	MET	2.5
1	F	183	ALA	2.5
1	I	211	ALA	2.5
1	I	104	LEU	2.5
1	D	236	THR	2.5
1	L	116	LYS	2.5
1	E	183	ALA	2.4
1	K	199	GLY	2.4
1	D	141	LEU	2.4
1	C	219	VAL	2.4
1	E	6	VAL	2.4
1	E	263	THR	2.4
1	K	45	ASP	2.4
1	K	85	SER	2.4
1	A	228	GLU	2.4
1	G	260	TYR	2.4
1	E	26	ILE	2.4
1	K	262	GLU	2.4
1	E	104	LEU	2.4
1	D	221	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	2.4
1	A	198	GLY	2.4
1	I	234	ALA	2.4
1	J	180	ILE	2.4
1	K	113	ALA	2.4
1	F	135	LYS	2.4
1	C	67	LEU	2.4
1	E	74	PHE	2.4
1	K	47	ALA	2.4
1	D	5	LEU	2.4
1	E	103	PHE	2.4
1	A	183	ALA	2.3
1	J	230	ALA	2.3
1	K	36	VAL	2.3
1	C	226	GLU	2.3
1	E	116	LYS	2.3
1	F	31	GLU	2.3
1	F	222	GLU	2.3
1	H	16	GLU	2.3
1	C	184	THR	2.3
1	D	67	LEU	2.3
1	C	7	ILE	2.3
1	E	124	LYS	2.3
1	K	13	ILE	2.3
1	G	200	MET	2.3
1	L	189	LEU	2.3
1	K	4	PHE	2.3
1	E	8	ALA	2.3
1	K	24	GLU	2.3
1	E	192	GLY	2.3
1	I	197	SER	2.3
1	K	238	LEU	2.3
1	G	191	GLY	2.3
1	E	123	VAL	2.3
1	K	132	TRP	2.3
1	F	73	GLU	2.3
1	K	222	GLU	2.3
1	D	65	LYS	2.3
1	B	20	LEU	2.3
1	E	95	ALA	2.3
1	L	234	ALA	2.3
1	D	61	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	61	GLU	2.3
1	L	86	TRP	2.3
1	C	227	PRO	2.3
1	E	101	PRO	2.3
1	E	235	PRO	2.3
1	F	90	PRO	2.3
1	I	152	THR	2.3
1	E	119	ARG	2.3
1	K	114	ALA	2.3
1	C	232	SER	2.2
1	L	218	GLY	2.2
1	I	200	MET	2.2
1	K	14	GLU	2.2
1	D	182	ASP	2.2
1	F	26	ILE	2.2
1	J	185	HIS	2.2
1	D	76	LEU	2.2
1	A	80	THR	2.2
1	C	15	SER	2.2
1	K	145	GLY	2.2
1	F	226	GLU	2.2
1	D	207	LEU	2.2
1	B	152	THR	2.2
1	E	241	SER	2.2
1	D	92	ALA	2.2
1	E	47	ALA	2.2
1	I	233	ASP	2.2
1	L	35	GLU	2.2
1	E	184	THR	2.2
1	K	3	LYS	2.2
1	C	6	VAL	2.2
1	F	22	VAL	2.2
1	F	122	ASN	2.2
1	F	124	LYS	2.2
1	F	142	LYS	2.2
1	K	5	LEU	2.2
1	E	132	TRP	2.2
1	L	152	THR	2.2
1	J	191	GLY	2.2
1	K	9	GLY	2.2
1	L	226	GLU	2.2
1	L	228	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	65	LYS	2.2
1	L	101	PRO	2.2
1	E	243	LEU	2.1
1	J	207	LEU	2.1
1	E	51	SER	2.1
1	G	184	THR	2.1
1	L	199	GLY	2.1
1	B	102	ALA	2.1
1	E	64	VAL	2.1
1	K	121	VAL	2.1
1	K	42	SER	2.1
1	D	111	LEU	2.1
1	F	231	LEU	2.1
1	G	196	LYS	2.1
1	K	43	SER	2.1
1	L	85	SER	2.1
1	D	29	LEU	2.1
1	D	91	VAL	2.1
1	E	42	SER	2.1
1	A	180	ILE	2.1
1	L	82	ILE	2.1
1	L	124	LYS	2.1
1	L	110	LEU	2.1
1	K	225	PRO	2.1
1	G	198	GLY	2.1
1	G	262	GLU	2.1
1	J	186	SER	2.1
1	D	86	TRP	2.1
1	E	100	ILE	2.1
1	H	231	LEU	2.1
1	F	102	ALA	2.1
1	F	116	LYS	2.1
1	K	88	ALA	2.1
1	B	186	SER	2.1
1	E	181	TYR	2.1
1	B	184	THR	2.0
1	F	80	THR	2.0
1	H	79	THR	2.0
1	I	195	ASP	2.1
1	F	244	GLU	2.0
1	D	26	ILE	2.0
1	D	190	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	18	LEU	2.0
1	E	48	ASN	2.0
1	E	60	LEU	2.0
1	K	175	GLN	2.0
1	I	199	GLY	2.0
1	F	15	SER	2.0
1	K	66	ALA	2.0
1	E	138	VAL	2.0
1	I	219	VAL	2.0
1	C	52	ILE	2.0
1	C	100	ILE	2.0
1	L	97	ILE	2.0
1	L	61	GLU	2.0
1	D	116	LYS	2.0
1	F	103	PHE	2.0
1	H	152	THR	2.0
1	L	74	PHE	2.0
1	B	196	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	PEP	C	268	10/10	0.92	0.23	0.69	52,58,65,65	0
2	PEP	H	268	10/10	0.93	0.20	0.48	41,46,48,49	0
2	PEP	E	268	10/10	0.93	0.27	0.39	63,66,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	A5P	L	269	14/14	0.66	0.32	0.33	77,78,79,79	0
2	PEP	L	268	10/10	0.90	0.23	0.32	61,65,66,66	0
3	A5P	G	269	14/14	0.89	0.20	0.32	38,45,48,51	0
3	A5P	A	269	14/14	0.95	0.18	0.09	36,46,51,54	0
3	A5P	J	269	14/14	0.90	0.19	0.04	35,42,47,48	0
4	1NT	D	268	25/25	0.84	0.23	-0.05	59,64,67,68	0
2	PEP	I	268	10/10	0.95	0.18	-0.06	32,41,45,45	0
3	A5P	F	269	14/14	0.83	0.24	-0.08	77,81,84,85	0
2	PEP	J	268	10/10	0.94	0.20	-0.09	36,39,40,42	0
3	A5P	K	269	14/14	0.77	0.24	-0.13	72,74,75,75	0
3	A5P	B	269	14/14	0.93	0.17	-0.19	35,40,45,47	0
2	PEP	G	268	10/10	0.93	0.18	-0.22	35,39,43,43	0
3	A5P	H	269	14/14	0.93	0.18	-0.23	41,49,56,58	0
2	PEP	B	268	10/10	0.95	0.18	-0.27	31,37,39,40	0
3	A5P	E	269	14/14	0.83	0.22	-0.28	70,72,73,74	0
2	PEP	K	268	10/10	0.94	0.22	-0.29	67,70,74,74	0
3	A5P	I	269	14/14	0.93	0.16	-0.35	35,40,47,47	0
2	PEP	F	268	10/10	0.90	0.21	-0.44	62,66,71,72	0
3	A5P	C	269	14/14	0.88	0.17	-0.64	53,61,64,65	0
2	PEP	A	268	10/10	0.96	0.14	-1.47	30,34,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.