



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:12 AM UTC

PDB ID : 1HFB / pdb_00001hfb
Title : Crystal structure of the tyrosine-regulated 3-deoxy-D-arabino-heptulosonate-7-phosphate synthase from *Saccharomyces cerevisiae* complexed with phosphoenolpyruvate
Authors : Schneider, T.R.; Hartmann, M.; Braus, G.H.
Deposited on : 2000-11-30
Resolution : 1.90 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

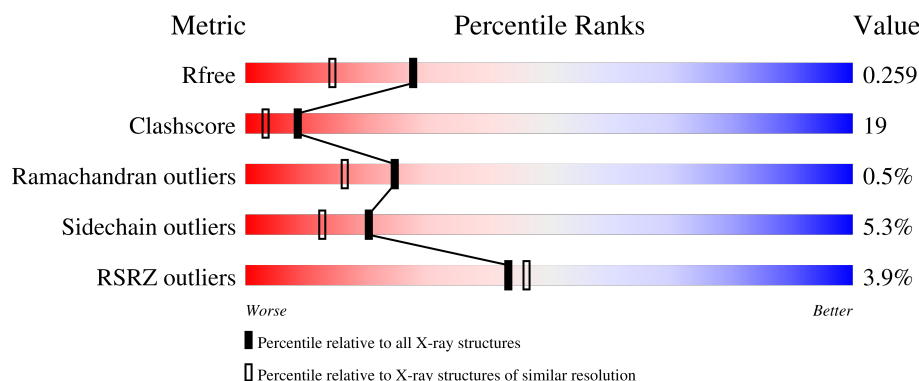
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	370	2% 63% 24% 5% 8%
1	B	370	2% 62% 25% • 9%
1	C	370	5% 59% 32% • 6%
1	D	370	2% 65% 25% • 8%
1	E	370	6% 52% 34% 5% 9%

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Mol	Chain	Length	Quality of chain
1	F	370	2%64%27%6%
1	G	370	8%52%35%6%8%
1	H	370	2%61%26%5%8%

2 Entry composition

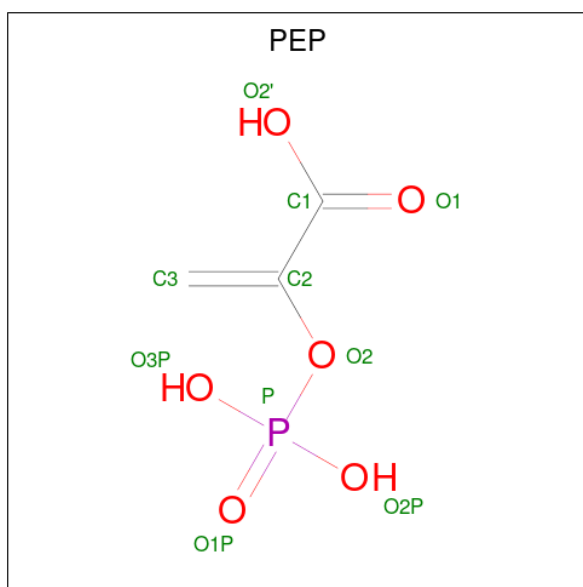
There are 3 unique types of molecules in this entry. The entry contains 21955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2568	1599	463	496	10			
1	B	336	Total	C	N	O	S	0	0	0
			2547	1586	459	492	10			
1	C	348	Total	C	N	O	S	0	0	0
			2629	1637	474	508	10			
1	D	342	Total	C	N	O	S	0	0	0
			2586	1610	467	499	10			
1	E	335	Total	C	N	O	S	0	0	0
			2538	1580	457	491	10			
1	F	346	Total	C	N	O	S	0	0	0
			2610	1625	470	505	10			
1	G	342	Total	C	N	O	S	0	0	0
			2583	1609	465	499	10			
1	H	339	Total	C	N	O	S	0	0	0
			2563	1595	462	496	10			

- Molecule 2 is PHOSPHOENOLPYRUVATE (CCD ID: 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	D	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	187	Total	O	0	0
			187	187		
3	B	204	Total	O	0	0
			204	204		
3	C	142	Total	O	0	0
			142	142		
3	D	207	Total	O	0	0
			207	207		

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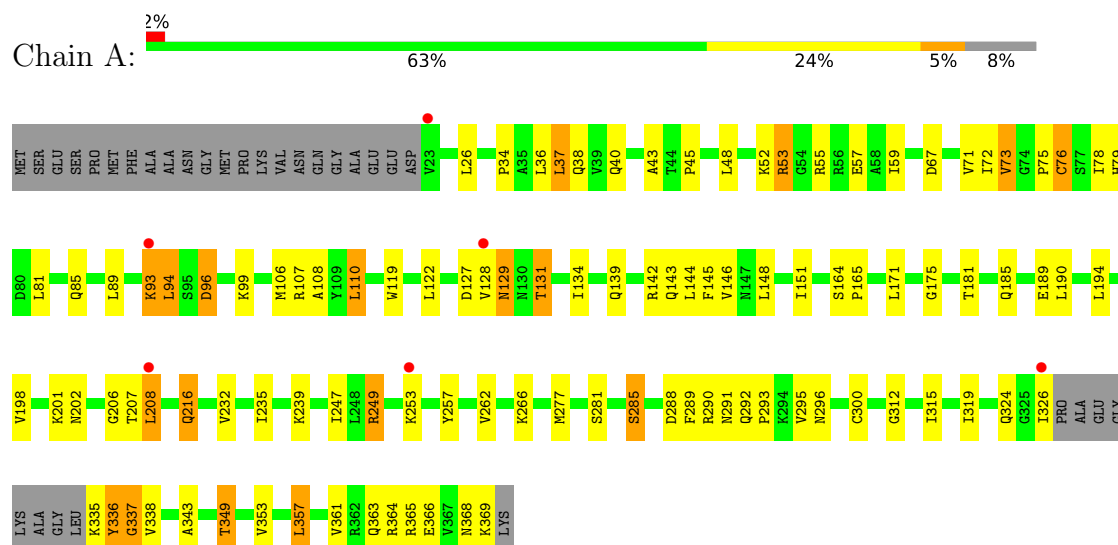
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	101	Total 101	O 101	0	0
3	F	168	Total 168	O 168	0	0
3	G	99	Total 99	O 99	0	0
3	H	143	Total 143	O 143	0	0

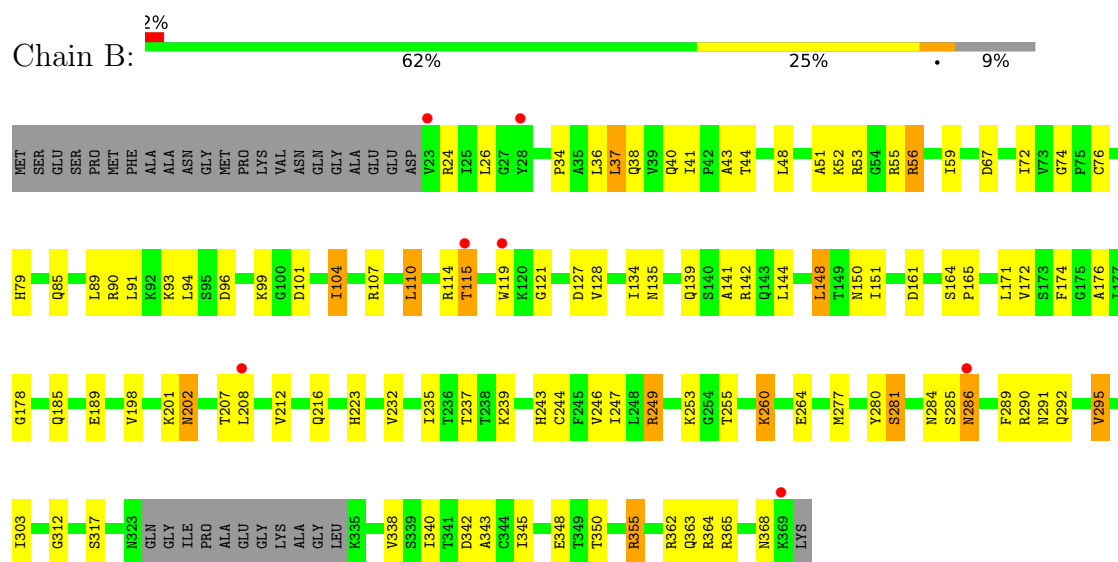
3 Residue-property plots [i](#)

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.

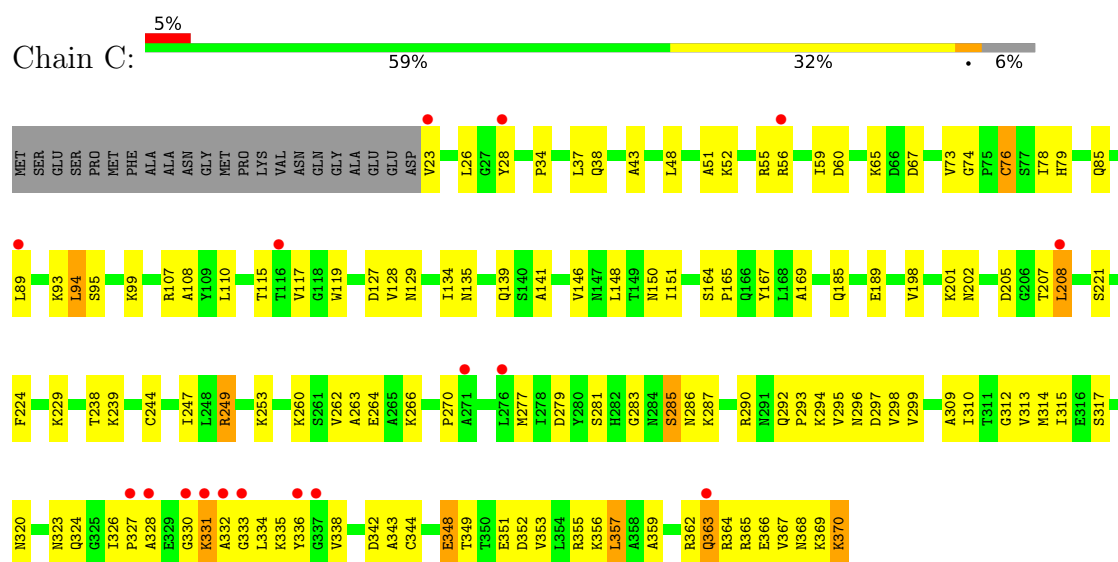
• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE



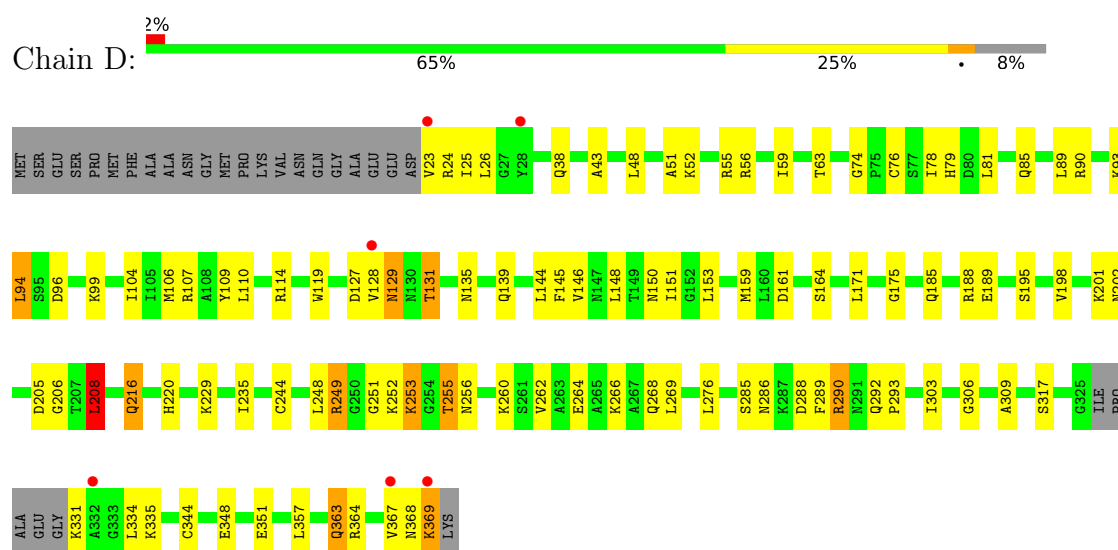
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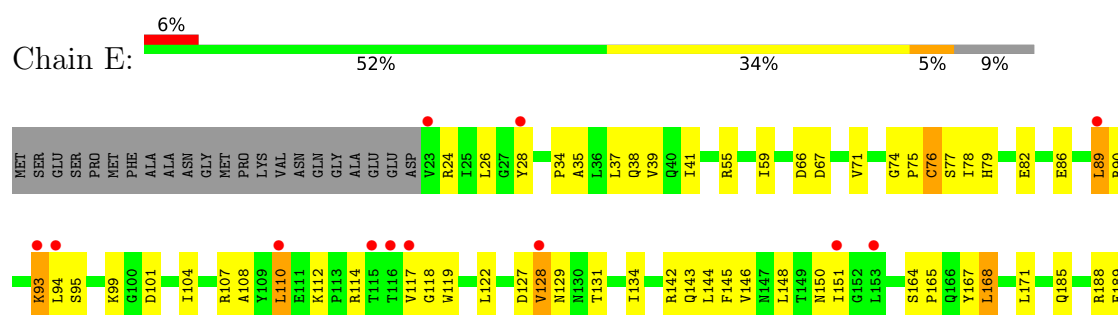
• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE

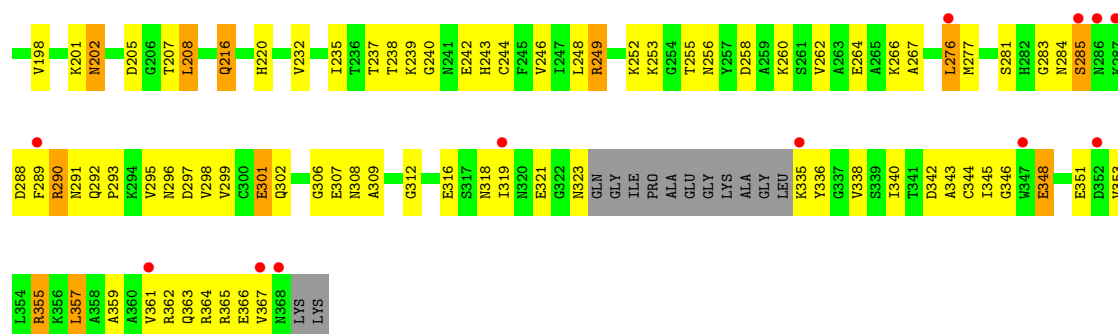


• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE

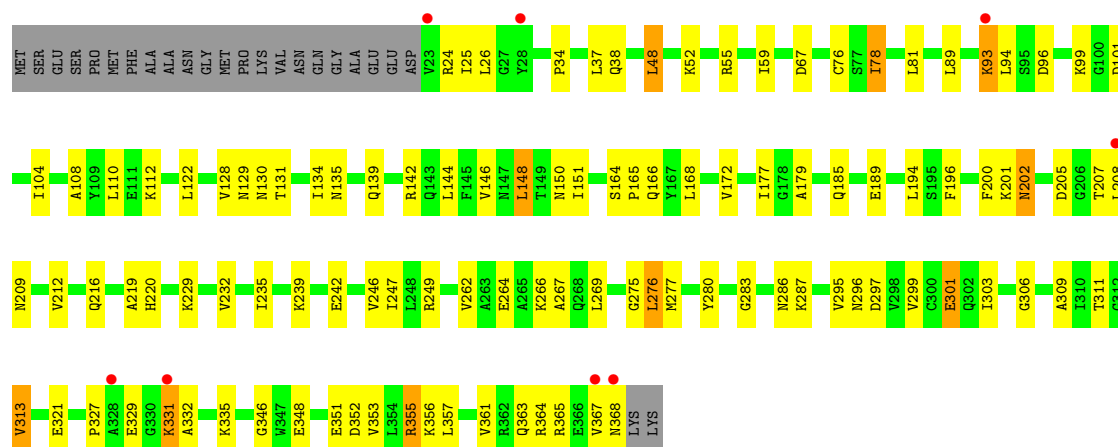


• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE

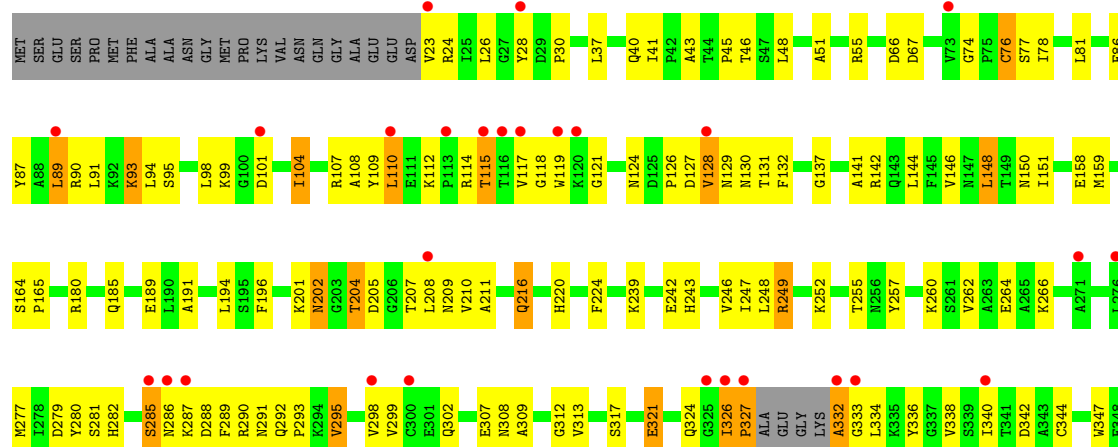


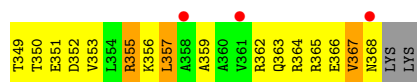


• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE

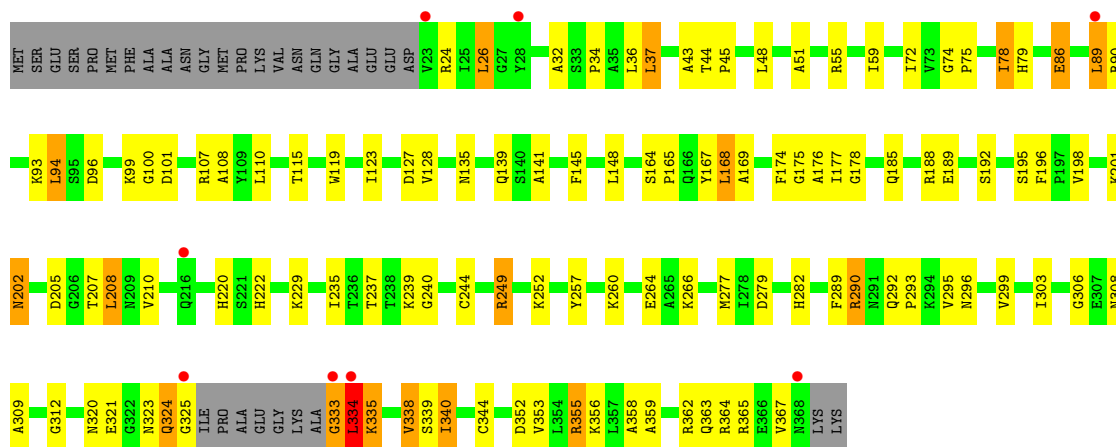


• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE





• Molecule 1: TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.00Å 93.80Å 104.50Å 65.60° 85.60° 75.40°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (40.00-1.90) 91.7 (40.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.261 0.205 , 0.259	Depositor DCC
R_{free} test set	10431 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21955	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 23.72 % 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 4.4095e-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: 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	0/2605	0.94	5/3525 (0.1%)
1	B	0.42	0/2584	0.92	7/3497 (0.2%)
1	C	0.41	0/2668	0.95	4/3609 (0.1%)
1	D	0.42	0/2623	0.92	5/3548 (0.1%)
1	E	0.40	0/2575	0.92	6/3486 (0.2%)
1	F	0.41	0/2649	0.95	4/3587 (0.1%)
1	G	0.42	0/2622	0.94	8/3552 (0.2%)
1	H	0.43	0/2601	1.00	10/3522 (0.3%)
All	All	0.42	0/20927	0.94	49/28326 (0.2%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	334	LEU	N-CA-C	14.25	141.16	110.80
1	G	326	ILE	N-CA-C	8.79	117.01	107.60
1	A	285	SER	N-CA-C	-7.71	103.88	113.28
1	H	335	LYS	N-CA-C	-7.34	97.73	109.76
1	H	334	LEU	CA-C-N	7.31	133.54	122.65
1	H	334	LEU	C-N-CA	7.31	133.54	122.65
1	G	76	CYS	N-CA-C	-7.06	103.51	111.14
1	G	295	VAL	N-CA-C	-6.96	104.20	111.58
1	G	326	ILE	CA-C-N	6.86	128.41	119.84
1	G	326	ILE	C-N-CA	6.86	128.41	119.84
1	A	76	CYS	N-CA-C	-6.78	103.97	111.36
1	B	104	ILE	N-CA-C	6.55	118.02	108.58
1	D	104	ILE	N-CA-C	6.51	117.95	108.58
1	E	104	ILE	N-CA-C	6.38	117.48	108.36
1	G	285	SER	N-CA-C	-6.29	105.09	112.89
1	F	104	ILE	N-CA-C	6.26	117.32	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	104	ILE	N-CA-C	6.20	116.85	108.17
1	C	76	CYS	N-CA-C	-6.06	104.75	111.36
1	B	295	VAL	N-CA-C	-6.04	104.62	110.72
1	A	131	THR	N-CA-C	-6.01	106.27	113.97
1	B	178	GLY	N-CA-C	5.95	118.88	112.33
1	B	115	THR	N-CA-C	-5.86	105.03	111.82
1	E	188	ARG	N-CA-C	-5.70	105.15	111.36
1	H	340	ILE	N-CA-C	-5.69	106.76	112.17
1	A	94	LEU	N-CA-C	-5.47	105.70	112.38
1	C	328	ALA	N-CA-C	-5.45	105.49	111.82
1	D	256	ASN	N-CA-C	5.43	117.83	110.06
1	B	121	GLY	N-CA-C	5.42	117.87	111.63
1	C	285	SER	N-CA-C	-5.37	106.23	112.89
1	F	76	CYS	N-CA-C	-5.37	105.43	111.28
1	B	172	VAL	N-CA-C	5.33	115.98	108.36
1	E	76	CYS	N-CA-C	-5.32	105.48	111.28
1	F	172	VAL	N-CA-C	5.32	115.97	108.36
1	E	208	LEU	N-CA-C	5.30	118.91	112.23
1	H	169	ALA	N-CA-C	5.30	117.74	111.33
1	G	333	GLY	N-CA-C	-5.27	100.68	113.18
1	C	169	ALA	N-CA-C	5.24	117.67	111.33
1	H	188	ARG	N-CA-C	-5.21	105.67	112.23
1	D	131	THR	N-CA-C	-5.20	107.31	113.97
1	E	285	SER	N-CA-C	-5.20	106.44	112.89
1	A	79	HIS	N-CA-C	-5.20	106.85	114.39
1	E	71	VAL	N-CA-C	5.16	115.48	107.28
1	F	122	LEU	N-CA-C	5.15	116.89	111.28
1	H	94	LEU	N-CA-C	-5.12	105.70	111.28
1	B	345	ILE	N-CA-C	-5.12	104.47	110.05
1	H	115	THR	N-CA-C	-5.08	105.74	111.28
1	D	76	CYS	N-CA-C	-5.08	105.75	111.28
1	D	208	LEU	N-CA-C	5.07	118.50	112.72
1	H	178	GLY	N-CA-C	5.04	117.72	111.93

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	2568	0	2587	84	0
1	B	2547	0	2565	85	0
1	C	2629	0	2654	108	0
1	D	2586	0	2608	90	0
1	E	2538	0	2552	128	0
1	F	2610	0	2628	87	0
1	G	2583	0	2601	143	0
1	H	2563	0	2578	107	0
2	A	10	0	2	0	0
2	B	10	0	2	0	0
2	C	10	0	2	0	0
2	D	10	0	2	0	0
2	E	10	0	2	0	0
2	F	10	0	2	3	0
2	G	10	0	2	0	0
2	H	10	0	2	1	0
3	A	187	0	0	8	0
3	B	204	0	0	6	0
3	C	142	0	0	6	0
3	D	207	0	0	12	0
3	E	101	0	0	4	0
3	F	168	0	0	7	0
3	G	99	0	0	8	0
3	H	143	0	0	6	0
All	All	21955	0	20789	786	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 19.

All (786) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD11	1:B:246:VAL:HG11	1.38	1.05
1:G:93:LYS:HD3	1:G:94:LEU:N	1.79	0.98
1:F:208:LEU:HD11	1:F:246:VAL:HG11	1.47	0.95
1:A:76:CYS:HB2	3:A:2170:HOH:O	1.65	0.94
1:G:355:ARG:HH11	1:G:355:ARG:HG3	1.32	0.93
1:B:37:LEU:HD12	1:B:142:ARG:HD3	1.51	0.92
1:E:348:GLU:CD	1:E:348:GLU:H	1.75	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:LYS:HD2	1:H:94:LEU:N	1.86	0.91
1:D:208:LEU:H	1:D:208:LEU:HD12	1.36	0.90
1:E:290:ARG:HH11	1:E:290:ARG:HB2	1.37	0.89
1:E:93:LYS:HD3	1:E:94:LEU:N	1.88	0.89
1:A:53:ARG:HD2	1:A:57:GLU:OE2	1.73	0.88
1:A:71:VAL:HG12	1:A:73:VAL:HG22	1.57	0.86
1:C:76:CYS:SG	1:C:342:ASP:HB2	2.16	0.85
1:F:185:GLN:O	1:F:189:GLU:HG3	1.78	0.83
1:A:93:LYS:HD3	1:A:94:LEU:N	1.93	0.83
1:G:208:LEU:HD11	1:G:246:VAL:HG11	1.65	0.79
1:G:76:CYS:SG	1:G:342:ASP:HB2	2.23	0.78
1:H:185:GLN:O	1:H:189:GLU:HG3	1.84	0.78
1:E:252:LYS:HE3	1:F:207:THR:HG21	1.66	0.78
1:H:290:ARG:HH11	1:H:290:ARG:HB2	1.49	0.78
1:H:78:ILE:HD13	1:H:108:ALA:HA	1.64	0.77
1:A:73:VAL:HG13	1:A:315:ILE:HB	1.66	0.77
1:A:110:LEU:HD21	1:A:145:PHE:CE1	2.20	0.77
1:B:43:ALA:HB3	1:B:48:LEU:HD21	1.67	0.77
1:G:185:GLN:O	1:G:189:GLU:HG3	1.84	0.76
1:G:364:ARG:O	1:G:367:VAL:HG22	1.85	0.76
1:A:48:LEU:O	1:A:52:LYS:HD3	1.85	0.76
1:D:369:LYS:HG3	3:D:2204:HOH:O	1.85	0.76
1:G:202:ASN:HB2	1:G:207:THR:O	1.86	0.76
1:H:89:LEU:HG	1:H:90:ARG:N	2.00	0.76
1:B:37:LEU:CD1	1:B:142:ARG:HD3	2.15	0.76
1:G:349:THR:O	1:G:353:VAL:HG23	1.86	0.75
1:F:93:LYS:HD3	1:F:94:LEU:N	2.01	0.75
1:A:81:LEU:HD22	1:A:144:LEU:HD13	1.67	0.74
1:E:114:ARG:NH1	1:E:118:GLY:HA3	2.02	0.74
1:F:269:LEU:HD11	1:F:276:LEU:HD13	1.70	0.74
1:B:348:GLU:HG3	3:B:2194:HOH:O	1.87	0.74
1:F:78:ILE:HD13	1:F:108:ALA:HA	1.69	0.74
1:E:260:LYS:HZ3	1:E:264:GLU:HG2	1.52	0.73
1:A:36:LEU:O	1:A:40:GLN:HG3	1.88	0.73
1:C:348:GLU:CD	1:C:348:GLU:H	1.94	0.73
1:D:78:ILE:HG12	3:D:2059:HOH:O	1.88	0.73
1:B:93:LYS:HG3	1:B:94:LEU:N	2.04	0.73
1:F:249:ARG:HD2	2:F:500:PEP:O3P	1.89	0.72
1:C:359:ALA:HA	1:C:362:ARG:HE	1.53	0.72
1:H:324:GLN:HE21	1:H:338:VAL:HG22	1.53	0.72
1:D:93:LYS:HD2	1:D:94:LEU:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LYS:HE2	1:F:24:ARG:HG2	1.72	0.72
1:E:185:GLN:O	1:E:189:GLU:HG3	1.90	0.71
1:A:216:GLN:HE21	1:A:216:GLN:HA	1.54	0.71
1:C:330:GLY:C	1:C:332:ALA:H	1.97	0.71
1:H:79:HIS:CE1	1:H:334:LEU:HD13	2.26	0.71
1:A:185:GLN:O	1:A:189:GLU:HG3	1.91	0.71
1:A:239:LYS:HG2	1:B:24:ARG:HA	1.73	0.71
1:E:288:ASP:HB3	1:E:291:ASN:ND2	2.06	0.70
1:F:331:LYS:HD2	1:F:332:ALA:N	2.06	0.70
1:H:320:ASN:HB2	1:H:338:VAL:HG12	1.72	0.70
1:H:266:LYS:HD3	1:H:309:ALA:CB	2.21	0.70
1:E:110:LEU:HD21	1:E:145:PHE:CE1	2.27	0.70
1:F:331:LYS:HD2	1:F:332:ALA:H	1.57	0.69
1:E:232:VAL:HG12	1:F:232:VAL:HG12	1.74	0.69
1:G:77:SER:HB3	1:G:112:LYS:HD2	1.73	0.69
1:C:331:LYS:HA	1:C:334:LEU:HD21	1.73	0.69
1:E:146:VAL:O	1:E:150:ASN:HB2	1.93	0.69
1:E:364:ARG:O	1:E:367:VAL:HG22	1.93	0.69
1:B:208:LEU:HD11	1:B:246:VAL:CG1	2.19	0.69
1:G:355:ARG:HG3	1:G:355:ARG:NH1	2.07	0.69
1:B:93:LYS:HG3	1:B:94:LEU:H	1.58	0.69
1:H:79:HIS:HE1	1:H:334:LEU:HD13	1.57	0.69
1:D:119:TRP:CE2	1:D:128:VAL:HG12	2.28	0.69
1:H:324:GLN:NE2	1:H:338:VAL:HG22	2.07	0.69
1:E:26:LEU:CD2	1:F:239:LYS:HB3	2.23	0.68
1:H:205:ASP:HA	1:H:252:LYS:HD3	1.75	0.68
1:H:334:LEU:HD23	1:H:334:LEU:H	1.59	0.68
1:F:262:VAL:O	1:F:266:LYS:HG3	1.93	0.68
1:G:281:SER:HA	1:G:285:SER:HB2	1.76	0.68
1:H:324:GLN:HG2	1:H:338:VAL:CG2	2.24	0.68
1:C:295:VAL:O	1:C:299:VAL:HG23	1.94	0.67
1:C:281:SER:HA	1:C:285:SER:HB3	1.76	0.67
1:G:363:GLN:O	1:G:367:VAL:HG13	1.94	0.67
1:A:324:GLN:OE1	1:A:335:LYS:HB2	1.95	0.67
1:H:323:ASN:HA	1:H:339:SER:O	1.95	0.67
1:C:56:ARG:HD2	3:C:2014:HOH:O	1.93	0.67
1:C:239:LYS:HE2	1:D:24:ARG:HG2	1.76	0.66
1:E:266:LYS:HD3	1:E:309:ALA:CB	2.25	0.66
1:A:129:ASN:C	1:A:129:ASN:HD22	2.04	0.66
1:B:55:ARG:O	1:B:59:ILE:HG13	1.95	0.66
1:C:60:ASP:OD1	1:C:65:LYS:HE2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LYS:HG2	1:F:24:ARG:HA	1.77	0.66
1:D:364:ARG:O	1:D:367:VAL:HG22	1.96	0.66
1:E:262:VAL:O	1:E:266:LYS:HG3	1.96	0.66
1:H:324:GLN:OE1	1:H:334:LEU:HA	1.95	0.66
1:A:110:LEU:HD21	1:A:145:PHE:HE1	1.60	0.66
1:C:260:LYS:O	1:C:264:GLU:HG3	1.97	0.65
1:F:208:LEU:HD11	1:F:246:VAL:CG1	2.25	0.65
1:A:110:LEU:HD12	1:A:122:LEU:HD23	1.79	0.65
1:C:317:SER:HA	1:C:344:CYS:HB3	1.76	0.65
1:G:202:ASN:C	1:G:202:ASN:HD22	2.04	0.65
1:D:51:ALA:O	1:D:55:ARG:HG3	1.96	0.65
1:F:166:GLN:OE1	1:F:229:LYS:HE3	1.96	0.65
1:B:239:LYS:HE3	3:B:2133:HOH:O	1.96	0.65
1:E:110:LEU:HD22	1:E:110:LEU:N	2.12	0.65
1:E:335:LYS:O	1:E:338:VAL:HG12	1.97	0.64
1:C:78:ILE:HD13	1:C:108:ALA:HA	1.78	0.64
1:B:56:ARG:HH11	1:B:56:ARG:HB2	1.61	0.64
1:C:85:GLN:O	1:C:89:LEU:HD13	1.98	0.64
1:D:90:ARG:O	1:D:93:LYS:HG3	1.97	0.64
1:G:159:MET:HE2	1:G:196:PHE:HZ	1.61	0.64
1:C:134:ILE:HD12	1:D:235:ILE:HG23	1.79	0.64
1:H:364:ARG:O	1:H:367:VAL:HG22	1.98	0.64
1:F:78:ILE:HD12	3:F:2023:HOH:O	1.97	0.64
1:B:85:GLN:O	1:B:89:LEU:HD23	1.97	0.64
1:F:269:LEU:HD11	1:F:276:LEU:CD1	2.28	0.64
1:D:348:GLU:H	1:D:348:GLU:CD	2.06	0.63
1:B:208:LEU:CD1	1:B:246:VAL:HG11	2.24	0.63
1:E:142:ARG:HD3	1:E:167:TYR:O	1.98	0.63
1:H:78:ILE:HD12	3:H:2023:HOH:O	1.98	0.63
1:B:119:TRP:NE1	1:B:128:VAL:HG12	2.13	0.63
1:D:368:ASN:O	1:D:369:LYS:O	2.15	0.63
1:B:36:LEU:O	1:B:40:GLN:HG3	1.98	0.63
1:E:34:PRO:O	1:E:38:GLN:HG3	1.99	0.63
1:D:48:LEU:O	1:D:52:LYS:HD3	1.99	0.63
1:E:110:LEU:HD21	1:E:145:PHE:CZ	2.34	0.63
1:B:79:HIS:HD2	3:B:2024:HOH:O	1.81	0.63
1:D:208:LEU:HD12	1:D:208:LEU:N	2.08	0.62
1:A:262:VAL:O	1:A:266:LYS:HG3	1.99	0.62
1:D:43:ALA:HB3	1:D:48:LEU:HD21	1.81	0.62
1:E:296:ASN:ND2	1:E:353:VAL:HG13	2.14	0.62
1:A:281:SER:HA	1:A:285:SER:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HG2	1:A:368:ASN:HD21	1.64	0.62
1:E:290:ARG:HH11	1:E:290:ARG:CB	2.09	0.62
1:G:45:PRO:HG2	3:G:2011:HOH:O	1.99	0.62
1:F:48:LEU:O	1:F:52:LYS:HD3	2.00	0.62
1:H:93:LYS:HD2	1:H:94:LEU:H	1.64	0.62
1:C:296:ASN:ND2	1:C:353:VAL:HG13	2.14	0.62
1:F:96:ASP:O	1:F:99:LYS:HG2	1.99	0.62
1:D:119:TRP:NE1	1:D:128:VAL:HG12	2.15	0.61
1:H:101:ASP:HA	1:H:365:ARG:HH22	1.65	0.61
1:A:110:LEU:N	1:A:110:LEU:HD22	2.16	0.61
1:A:129:ASN:ND2	1:A:131:THR:HG23	2.14	0.61
1:C:313:VAL:HG21	1:C:357:LEU:HD11	1.83	0.61
1:G:291:ASN:O	1:G:295:VAL:HG23	2.01	0.61
1:D:55:ARG:O	1:D:59:ILE:HG13	2.01	0.61
1:B:119:TRP:CE2	1:B:128:VAL:HG12	2.36	0.61
1:E:55:ARG:O	1:E:59:ILE:HG13	2.00	0.61
1:G:114:ARG:NH1	1:G:118:GLY:HA3	2.16	0.61
1:H:289:PHE:CZ	1:H:290:ARG:HD2	2.36	0.61
1:H:324:GLN:HG2	1:H:338:VAL:HG23	1.83	0.60
1:A:128:VAL:HG23	1:A:128:VAL:O	2.00	0.60
1:A:134:ILE:HD12	1:B:235:ILE:HG23	1.83	0.60
1:A:266:LYS:HE2	3:A:2147:HOH:O	2.02	0.60
1:E:26:LEU:HD23	1:F:239:LYS:HB3	1.82	0.60
1:E:110:LEU:HD11	1:E:144:LEU:HD23	1.82	0.60
1:H:55:ARG:O	1:H:59:ILE:HG13	2.01	0.60
1:G:40:GLN:NE2	3:G:2009:HOH:O	2.33	0.60
1:A:34:PRO:O	1:A:38:GLN:HG3	2.02	0.60
1:A:119:TRP:NE1	1:A:128:VAL:HG12	2.17	0.60
1:B:37:LEU:HD12	1:B:142:ARG:CD	2.30	0.60
1:G:204:THR:HB	3:G:2060:HOH:O	2.02	0.60
1:C:48:LEU:O	1:C:52:LYS:HD3	2.02	0.60
1:C:266:LYS:HD3	1:C:309:ALA:CB	2.32	0.60
1:C:370:LYS:HA	1:C:370:LYS:NZ	2.17	0.60
1:H:75:PRO:O	3:H:2024:HOH:O	2.16	0.60
1:C:78:ILE:CD1	1:C:108:ALA:HA	2.32	0.59
1:F:352:ASP:O	1:F:356:LYS:HG2	2.01	0.59
1:G:292:GLN:N	1:G:293:PRO:HD2	2.17	0.59
1:B:148:LEU:O	1:B:151:ILE:HG12	2.02	0.59
1:G:81:LEU:HG	1:G:144:LEU:HD13	1.85	0.59
1:G:41:ILE:HB	1:G:142:ARG:HD3	1.84	0.59
1:G:127:ASP:HB3	1:G:129:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:308:ASN:OD1	1:H:364:ARG:HD2	2.02	0.59
1:A:73:VAL:CG1	1:A:315:ILE:HB	2.32	0.59
1:B:37:LEU:HD21	1:B:139:GLN:HG2	1.84	0.59
1:D:23:VAL:HG23	1:D:25:ILE:H	1.68	0.59
1:E:235:ILE:HG23	1:F:134:ILE:HD12	1.85	0.59
1:D:208:LEU:HD11	1:D:268:GLN:NE2	2.18	0.59
1:H:303:ILE:O	1:H:364:ARG:HB2	2.03	0.59
1:G:207:THR:HG22	1:G:208:LEU:N	2.18	0.59
1:G:355:ARG:HH11	1:G:355:ARG:CG	2.10	0.59
1:A:143:GLN:O	1:A:146:VAL:HG22	2.03	0.59
1:B:185:GLN:O	1:B:189:GLU:HG3	2.02	0.59
1:C:94:LEU:HD13	1:C:94:LEU:O	2.02	0.59
1:G:260:LYS:O	1:G:264:GLU:HG3	2.02	0.58
1:A:296:ASN:CG	1:A:353:VAL:HG13	2.28	0.58
1:G:115:THR:HG22	1:G:180:ARG:HH21	1.67	0.58
1:B:53:ARG:HA	1:B:56:ARG:NH1	2.17	0.58
1:G:23:VAL:HG23	3:G:2001:HOH:O	2.01	0.58
1:G:67:ASP:CG	1:G:365:ARG:HH11	2.11	0.58
1:F:55:ARG:O	1:F:59:ILE:HG13	2.03	0.58
1:G:202:ASN:HD21	1:G:249:ARG:HE	1.52	0.58
1:C:262:VAL:O	1:C:266:LYS:HG3	2.04	0.58
1:C:370:LYS:HA	1:C:370:LYS:CE	2.34	0.58
1:D:128:VAL:HG22	1:D:331:LYS:HE2	1.85	0.58
1:G:164:SER:HB2	1:G:165:PRO:HD3	1.85	0.57
1:G:262:VAL:O	1:G:266:LYS:HG3	2.04	0.57
1:E:239:LYS:HB3	1:F:26:LEU:CD2	2.34	0.57
1:D:262:VAL:O	1:D:266:LYS:HG3	2.04	0.57
1:A:326:ILE:HD12	1:A:326:ILE:C	2.28	0.57
1:G:334:LEU:HD11	1:G:340:ILE:HD12	1.85	0.57
1:E:76:CYS:SG	1:E:342:ASP:HB2	2.45	0.57
1:G:67:ASP:OD2	1:G:365:ARG:HG2	2.03	0.57
1:C:119:TRP:NE1	1:C:128:VAL:HG12	2.19	0.57
1:E:167:TYR:C	1:E:168:LEU:HD13	2.30	0.57
1:G:119:TRP:CE2	1:G:128:VAL:HG12	2.39	0.57
1:A:291:ASN:O	1:A:295:VAL:HG23	2.05	0.57
1:F:81:LEU:HG	1:F:144:LEU:HD13	1.87	0.57
1:G:248:LEU:N	1:G:248:LEU:HD22	2.20	0.56
1:A:85:GLN:O	1:A:89:LEU:HD23	2.05	0.56
1:A:81:LEU:HD22	1:A:144:LEU:HB2	1.87	0.56
1:C:202:ASN:HB3	1:C:208:LEU:HD12	1.86	0.56
1:B:37:LEU:HD13	1:B:37:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:HG22	3:B:2091:HOH:O	2.04	0.56
1:G:110:LEU:CD2	1:G:141:ALA:HB1	2.36	0.56
1:D:334:LEU:HD12	1:D:334:LEU:O	2.05	0.56
1:E:129:ASN:OD1	1:E:131:THR:HG23	2.05	0.56
1:E:252:LYS:CE	1:F:207:THR:HG21	2.36	0.56
1:G:366:GLU:C	1:G:368:ASN:H	2.13	0.56
1:D:205:ASP:HA	1:D:252:LYS:CG	2.35	0.56
1:G:257:TYR:CG	1:G:295:VAL:HG13	2.40	0.56
1:E:296:ASN:CG	1:E:353:VAL:HG13	2.31	0.56
1:F:303:ILE:HG23	1:F:364:ARG:HD3	1.86	0.56
1:C:26:LEU:HD23	1:C:26:LEU:C	2.31	0.56
1:E:78:ILE:HD13	3:E:2012:HOH:O	2.06	0.56
1:G:201:LYS:HB3	1:G:249:ARG:HD2	1.88	0.56
1:E:276:LEU:HD13	1:E:276:LEU:H	1.70	0.55
1:E:288:ASP:OD1	1:E:290:ARG:HD3	2.06	0.55
1:F:205:ASP:CG	1:F:207:THR:HG23	2.32	0.55
1:H:43:ALA:HB3	1:H:48:LEU:HD21	1.88	0.55
1:D:185:GLN:O	1:D:189:GLU:HG3	2.06	0.55
1:C:296:ASN:CG	1:C:353:VAL:HG13	2.31	0.55
1:C:43:ALA:HB3	1:C:48:LEU:HD21	1.88	0.55
1:C:330:GLY:C	1:C:332:ALA:N	2.63	0.55
1:G:359:ALA:HA	1:G:362:ARG:HE	1.72	0.55
1:C:38:GLN:HE22	1:C:229:LYS:HD3	1.71	0.55
1:H:167:TYR:HB2	1:H:168:LEU:HD22	1.88	0.55
1:H:266:LYS:HD3	1:H:309:ALA:HB3	1.89	0.55
1:E:77:SER:HB3	1:E:112:LYS:HD3	1.88	0.55
1:G:90:ARG:HB3	1:G:347:TRP:CZ2	2.42	0.55
1:C:320:ASN:HB2	1:C:338:VAL:HG12	1.88	0.55
1:C:331:LYS:HA	1:C:334:LEU:CD2	2.36	0.55
1:E:101:ASP:OD1	1:E:365:ARG:NH2	2.40	0.55
1:F:179:ALA:HB2	1:F:249:ARG:HD3	1.89	0.55
1:B:281:SER:HA	1:B:285:SER:HB2	1.89	0.54
1:D:74:GLY:HA3	1:D:107:ARG:HB2	1.88	0.54
1:E:298:VAL:HA	1:E:301:GLU:HG2	1.89	0.54
1:F:327:PRO:HB2	1:F:329:GLU:CD	2.32	0.54
1:E:298:VAL:O	1:E:301:GLU:HG3	2.07	0.54
1:G:279:ASP:OD2	1:G:282:HIS:HD2	1.89	0.54
1:G:24:ARG:HD3	1:H:240:GLY:O	2.07	0.54
1:G:249:ARG:HH11	1:G:249:ARG:CG	2.20	0.54
1:A:201:LYS:HB3	1:A:249:ARG:HG2	1.90	0.54
1:C:331:LYS:CA	1:C:334:LEU:HD21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ALA:HA	1:E:362:ARG:NH1	2.21	0.54
1:C:23:VAL:HB	1:D:195:SER:OG	2.07	0.54
1:H:100:GLY:O	1:H:365:ARG:NH2	2.41	0.54
1:A:110:LEU:HB2	3:A:2068:HOH:O	2.08	0.54
1:A:349:THR:O	1:A:353:VAL:HG23	2.08	0.54
1:C:67:ASP:OD1	1:C:365:ARG:NH1	2.41	0.54
1:D:306:GLY:HA2	1:D:364:ARG:HG3	1.90	0.54
1:E:323:ASN:ND2	1:E:343:ALA:HB2	2.22	0.54
1:A:357:LEU:O	1:A:361:VAL:HG23	2.08	0.53
1:E:95:SER:O	1:E:99:LYS:HB3	2.08	0.53
1:A:119:TRP:CE2	1:A:128:VAL:HG12	2.44	0.53
1:B:364:ARG:HG2	1:B:368:ASN:ND2	2.22	0.53
1:E:357:LEU:O	1:E:361:VAL:HG23	2.08	0.53
1:C:352:ASP:O	1:C:356:LYS:HG3	2.09	0.53
1:F:348:GLU:HG3	3:F:2157:HOH:O	2.08	0.53
1:C:135:ASN:O	1:C:139:GLN:HG3	2.08	0.53
1:F:335:LYS:HG3	3:F:2149:HOH:O	2.07	0.53
1:B:96:ASP:O	1:B:99:LYS:HG2	2.08	0.53
1:B:303:ILE:O	1:B:364:ARG:HB2	2.09	0.53
1:G:207:THR:HG22	1:G:208:LEU:H	1.74	0.53
1:G:308:ASN:OD1	1:G:364:ARG:HD3	2.09	0.53
1:H:96:ASP:O	1:H:99:LYS:HG2	2.08	0.53
1:B:135:ASN:O	1:B:139:GLN:HG3	2.08	0.53
1:A:365:ARG:O	1:A:369:LYS:HG3	2.08	0.53
1:B:90:ARG:O	1:B:93:LYS:HG2	2.08	0.53
1:D:205:ASP:HA	1:D:252:LYS:HG2	1.91	0.53
1:E:39:VAL:HG21	1:G:30:PRO:HG3	1.91	0.53
1:F:129:ASN:O	1:F:130:ASN:HB2	2.08	0.53
1:H:295:VAL:O	1:H:299:VAL:HG23	2.09	0.53
1:H:324:GLN:HE22	1:H:335:LYS:H	1.57	0.53
1:C:201:LYS:HD3	1:C:247:ILE:HB	1.89	0.53
1:F:78:ILE:CD1	1:F:108:ALA:HA	2.39	0.53
1:G:257:TYR:CD1	1:G:295:VAL:HG13	2.44	0.53
1:E:301:GLU:HG3	1:E:302:GLN:N	2.24	0.52
1:G:159:MET:HE2	1:G:196:PHE:CZ	2.44	0.52
1:B:51:ALA:O	1:B:55:ARG:HG3	2.10	0.52
1:G:46:THR:HG23	3:G:2011:HOH:O	2.10	0.52
1:A:43:ALA:HB3	1:A:48:LEU:HD21	1.91	0.52
1:C:119:TRP:CE2	1:C:128:VAL:HG12	2.44	0.52
1:E:260:LYS:HZ3	1:E:264:GLU:CG	2.20	0.52
1:F:148:LEU:O	1:F:151:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:ASN:ND2	1:G:249:ARG:HE	2.06	0.52
1:H:260:LYS:O	1:H:264:GLU:HG3	2.09	0.52
1:C:52:LYS:O	1:C:56:ARG:HG3	2.09	0.52
1:F:219:ALA:HB2	3:F:2112:HOH:O	2.09	0.52
1:F:306:GLY:HA2	1:F:367:VAL:HG21	1.92	0.52
1:E:66:ASP:OD1	1:E:67:ASP:N	2.43	0.52
1:F:275:GLY:HA3	1:F:311:THR:OG1	2.09	0.52
1:H:279:ASP:OD2	1:H:282:HIS:HD2	1.92	0.52
1:D:129:ASN:ND2	1:D:129:ASN:H	2.08	0.52
1:D:260:LYS:O	1:D:264:GLU:HG3	2.10	0.52
1:F:129:ASN:OD1	1:F:131:THR:HG23	2.09	0.52
1:G:249:ARG:O	1:G:249:ARG:HG2	2.09	0.52
1:H:90:ARG:O	1:H:93:LYS:HE3	2.10	0.52
1:E:258:ASP:O	1:E:262:VAL:HG23	2.10	0.51
1:H:201:LYS:HD3	2:H:500:PEP:O2P	2.10	0.51
1:E:110:LEU:HD12	1:E:122:LEU:HD23	1.90	0.51
1:B:76:CYS:SG	1:B:342:ASP:HB2	2.50	0.51
1:G:110:LEU:HD21	1:G:141:ALA:HB1	1.92	0.51
1:F:364:ARG:O	1:F:367:VAL:HG22	2.10	0.51
1:A:45:PRO:HD2	3:A:2011:HOH:O	2.10	0.51
1:A:94:LEU:HD13	1:A:94:LEU:O	2.11	0.51
1:B:56:ARG:HH11	1:B:56:ARG:CB	2.24	0.51
1:B:364:ARG:HG2	1:B:368:ASN:HD21	1.74	0.51
1:D:129:ASN:ND2	1:D:131:THR:HG23	2.25	0.51
1:D:135:ASN:O	1:D:139:GLN:HG3	2.10	0.51
1:E:79:HIS:HB3	1:E:119:TRP:CH2	2.45	0.51
1:E:143:GLN:O	1:E:146:VAL:HG22	2.11	0.51
1:G:364:ARG:O	1:G:368:ASN:ND2	2.44	0.51
1:A:26:LEU:CD1	1:B:239:LYS:HB2	2.40	0.51
1:G:307:GLU:O	1:G:364:ARG:NH1	2.44	0.51
1:H:127:ASP:O	1:H:128:VAL:HG22	2.10	0.51
1:H:321:GLU:HA	1:H:344:CYS:O	2.10	0.51
1:A:78:ILE:HD13	3:A:2038:HOH:O	2.10	0.51
1:E:134:ILE:HD12	1:F:235:ILE:HG23	1.93	0.51
1:C:127:ASP:HB2	1:C:129:ASN:OD1	2.11	0.51
1:E:255:THR:HG22	1:E:284:ASN:HA	1.93	0.51
1:H:201:LYS:HB3	1:H:249:ARG:HG2	1.93	0.51
1:E:277:MET:HG3	1:E:312:GLY:C	2.36	0.50
1:G:26:LEU:CD2	1:H:239:LYS:HB2	2.40	0.50
1:G:180:ARG:NH1	3:G:2061:HOH:O	2.44	0.50
1:C:286:ASN:O	1:C:287:LYS:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLY:CA	1:D:107:ARG:HB2	2.41	0.50
1:E:82:GLU:OE1	1:E:82:GLU:N	2.34	0.50
1:G:93:LYS:HD3	1:G:94:LEU:CA	2.41	0.50
1:B:362:ARG:O	1:B:365:ARG:HB2	2.12	0.50
1:D:90:ARG:O	1:D:93:LYS:HE3	2.12	0.50
1:E:75:PRO:HB2	1:E:78:ILE:HD12	1.93	0.50
1:G:327:PRO:HG2	1:G:332:ALA:H	1.77	0.50
1:H:324:GLN:OE1	1:H:334:LEU:CA	2.60	0.50
1:C:117:VAL:HG11	1:D:220:HIS:CD2	2.47	0.50
1:F:202:ASN:HB2	1:F:207:THR:O	2.10	0.50
1:G:112:LYS:HE3	3:G:2050:HOH:O	2.12	0.50
1:B:53:ARG:HA	1:B:56:ARG:HH12	1.77	0.50
1:B:43:ALA:CB	1:B:48:LEU:HD21	2.40	0.50
1:C:323:ASN:HB3	1:C:343:ALA:HA	1.93	0.50
1:E:74:GLY:CA	1:E:107:ARG:HB2	2.41	0.50
1:E:168:LEU:N	1:E:168:LEU:HD22	2.27	0.50
1:E:216:GLN:O	1:E:220:HIS:HD2	1.95	0.50
1:C:351:GLU:O	1:C:355:ARG:HB2	2.11	0.50
1:F:78:ILE:CD1	3:F:2023:HOH:O	2.57	0.50
1:G:43:ALA:HB3	1:G:48:LEU:HD21	1.93	0.50
1:G:313:VAL:HG21	1:G:357:LEU:HD11	1.94	0.50
1:A:129:ASN:C	1:A:129:ASN:ND2	2.69	0.50
1:C:292:GLN:N	1:C:293:PRO:HD2	2.26	0.50
1:E:74:GLY:HA3	1:E:107:ARG:HB2	1.92	0.50
1:F:249:ARG:O	1:F:283:GLY:HA3	2.11	0.50
1:A:349:THR:HG21	3:A:2181:HOH:O	2.12	0.50
1:C:79:HIS:HD2	3:C:2027:HOH:O	1.95	0.50
1:D:26:LEU:HD13	1:D:26:LEU:C	2.37	0.50
1:G:86:GLU:O	1:G:89:LEU:HB2	2.12	0.50
1:G:334:LEU:CD1	1:G:340:ILE:HD12	2.42	0.50
1:A:206:GLY:O	1:A:253:LYS:HE2	2.12	0.49
1:D:38:GLN:HE22	1:D:229:LYS:NZ	2.10	0.49
1:D:334:LEU:HD12	1:D:334:LEU:C	2.37	0.49
1:G:78:ILE:HD13	1:G:108:ALA:HA	1.94	0.49
1:G:286:ASN:O	1:G:287:LYS:HB2	2.12	0.49
1:B:37:LEU:HD11	1:B:41:ILE:HD12	1.95	0.49
1:C:110:LEU:HD13	1:C:141:ALA:HB1	1.94	0.49
1:D:285:SER:O	1:D:286:ASN:HB2	2.12	0.49
1:F:286:ASN:O	1:F:287:LYS:HB2	2.12	0.49
1:C:366:GLU:OE2	1:C:369:LYS:HE3	2.11	0.49
1:H:45:PRO:HG2	3:H:2015:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ALA:O	1:H:55:ARG:HG3	2.11	0.49
1:F:55:ARG:HD3	1:F:196:PHE:HB3	1.94	0.49
1:C:370:LYS:HA	1:C:370:LYS:HE3	1.93	0.49
1:D:201:LYS:HD2	1:D:249:ARG:HG2	1.93	0.49
1:A:164:SER:N	1:A:165:PRO:CD	2.75	0.49
1:G:87:TYR:CD1	1:G:87:TYR:C	2.90	0.49
1:G:208:LEU:CD1	1:G:246:VAL:HG11	2.40	0.49
1:H:352:ASP:OD1	1:H:356:LYS:HE3	2.12	0.49
1:D:288:ASP:OD1	1:D:290:ARG:NH1	2.46	0.49
1:E:281:SER:HA	1:E:285:SER:HB2	1.93	0.49
1:H:192:SER:CB	1:H:222:HIS:HD2	2.25	0.49
1:E:117:VAL:HG11	1:F:220:HIS:CD2	2.48	0.49
1:E:145:PHE:HB3	1:E:171:LEU:HD13	1.95	0.49
1:F:295:VAL:O	1:F:299:VAL:HG23	2.12	0.49
1:A:364:ARG:HG2	1:A:368:ASN:ND2	2.28	0.49
1:F:351:GLU:HG2	1:F:355:ARG:HE	1.78	0.49
1:B:91:LEU:HD11	1:B:104:ILE:HG21	1.95	0.48
1:D:81:LEU:HG	1:D:144:LEU:HD13	1.94	0.48
1:E:264:GLU:O	1:E:267:ALA:HB3	2.13	0.48
1:G:28:TYR:HA	1:H:235:ILE:O	2.13	0.48
1:G:280:TYR:HE1	1:G:299:VAL:HG21	1.77	0.48
1:B:303:ILE:HG23	1:B:364:ARG:HD3	1.95	0.48
1:C:266:LYS:HD3	1:C:309:ALA:HB3	1.94	0.48
1:C:364:ARG:HD2	3:C:2139:HOH:O	2.13	0.48
1:F:212:VAL:O	1:F:216:GLN:HG2	2.13	0.48
1:G:366:GLU:O	1:G:368:ASN:N	2.46	0.48
1:C:349:THR:O	1:C:353:VAL:HG23	2.13	0.48
1:E:35:ALA:O	1:E:39:VAL:HG23	2.13	0.48
1:D:85:GLN:O	1:D:89:LEU:HD23	2.13	0.48
1:E:24:ARG:HA	1:F:239:LYS:HG2	1.96	0.48
1:D:94:LEU:HD11	1:D:351:GLU:HG3	1.95	0.48
1:E:79:HIS:HD2	3:E:2097:HOH:O	1.97	0.48
1:G:129:ASN:OD1	1:G:131:THR:HG23	2.13	0.48
1:G:355:ARG:NH1	1:G:355:ARG:CG	2.71	0.48
1:H:44:THR:O	1:H:48:LEU:HD23	2.13	0.48
1:B:212:VAL:O	1:B:216:GLN:HG2	2.14	0.48
1:D:129:ASN:H	1:D:129:ASN:HD22	1.60	0.48
1:D:335:LYS:HD2	1:D:335:LYS:HA	1.63	0.48
1:E:306:GLY:CA	1:E:367:VAL:HG21	2.43	0.48
1:G:66:ASP:OD1	1:G:67:ASP:N	2.46	0.48
1:A:208:LEU:N	1:A:208:LEU:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLY:HA3	1:B:107:ARG:HB2	1.95	0.48
1:D:106:MET:HB2	1:D:153:LEU:HD21	1.96	0.48
1:D:109:TYR:N	3:D:2059:HOH:O	2.47	0.48
1:D:306:GLY:CA	1:D:367:VAL:HG21	2.44	0.48
1:E:205:ASP:HA	1:E:252:LYS:HD3	1.96	0.48
1:E:292:GLN:HE21	1:E:345:ILE:HG23	1.78	0.48
1:E:298:VAL:O	1:E:302:GLN:HG3	2.13	0.48
1:G:249:ARG:CG	1:G:249:ARG:NH1	2.76	0.48
1:H:86:GLU:O	1:H:89:LEU:HD23	2.13	0.48
1:B:317:SER:HB2	1:B:350:THR:OG1	2.13	0.48
1:C:146:VAL:O	1:C:150:ASN:HB2	2.13	0.48
1:E:202:ASN:HB2	1:E:207:THR:O	2.14	0.48
1:F:242:GLU:C	3:F:2124:HOH:O	2.56	0.48
1:G:23:VAL:HB	1:H:195:SER:OG	2.13	0.48
1:A:300:CYS:SG	1:A:357:LEU:HA	2.54	0.48
1:A:235:ILE:HG23	1:B:134:ILE:HD12	1.96	0.47
1:B:260:LYS:O	1:B:264:GLU:HG3	2.14	0.47
1:B:290:ARG:NE	3:B:2165:HOH:O	2.47	0.47
1:E:37:LEU:HD23	1:E:167:TYR:HD2	1.79	0.47
1:B:72:ILE:HG22	1:B:107:ARG:HG3	1.96	0.47
1:D:363:GLN:NE2	3:D:2200:HOH:O	2.47	0.47
1:E:79:HIS:CD2	1:E:340:ILE:HG12	2.48	0.47
1:D:317:SER:HA	1:D:344:CYS:HB3	1.96	0.47
1:A:93:LYS:HD3	1:A:94:LEU:H	1.78	0.47
1:G:366:GLU:C	1:G:368:ASN:N	2.72	0.47
1:H:135:ASN:O	1:H:139:GLN:HG3	2.14	0.47
1:B:67:ASP:OD1	1:B:365:ARG:NH1	2.48	0.47
1:C:51:ALA:O	1:C:55:ARG:HG3	2.14	0.47
1:C:367:VAL:O	1:C:370:LYS:HG2	2.14	0.47
1:E:336:TYR:CD1	1:E:336:TYR:C	2.93	0.47
1:G:91:LEU:HD11	1:G:104:ILE:HG21	1.97	0.47
1:G:249:ARG:HG2	1:G:249:ARG:NH1	2.29	0.47
1:C:335:LYS:HB2	1:C:338:VAL:CG2	2.44	0.47
1:E:208:LEU:HD11	1:E:246:VAL:HG11	1.95	0.47
1:B:101:ASP:OD1	1:B:365:ARG:NH2	2.47	0.47
1:B:110:LEU:HD11	1:B:144:LEU:HD23	1.97	0.47
1:B:201:LYS:HD3	1:B:247:ILE:HB	1.97	0.47
1:C:324:GLN:OE1	1:C:334:LEU:HB2	2.15	0.47
1:E:78:ILE:HG21	1:E:144:LEU:HD22	1.95	0.47
1:E:318:ASN:O	1:E:319:ILE:C	2.58	0.47
1:F:112:LYS:NZ	2:F:500:PEP:O1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:ASP:O	1:F:301:GLU:HB2	2.14	0.47
1:G:201:LYS:HD3	1:G:247:ILE:HB	1.97	0.47
1:H:359:ALA:O	1:H:362:ARG:HB2	2.14	0.47
1:A:26:LEU:HD13	1:B:239:LYS:HB2	1.97	0.47
1:E:260:LYS:O	1:E:260:LYS:HD3	2.15	0.47
1:E:316:GLU:O	1:E:344:CYS:HB3	2.15	0.47
1:G:210:VAL:HG23	1:G:211:ALA:N	2.30	0.47
1:G:91:LEU:O	1:G:95:SER:HB2	2.14	0.47
1:G:146:VAL:O	1:G:150:ASN:HB2	2.15	0.47
1:H:119:TRP:CE2	1:H:128:VAL:HG12	2.50	0.47
1:C:331:LYS:H	1:C:331:LYS:HD2	1.80	0.47
1:E:351:GLU:OE2	1:E:355:ARG:NH1	2.47	0.47
1:G:127:ASP:HB3	1:G:129:ASN:HD21	1.80	0.47
1:G:288:ASP:OD1	1:G:290:ARG:HG3	2.14	0.47
1:B:90:ARG:O	1:B:93:LYS:CG	2.63	0.46
1:C:249:ARG:HD3	1:C:249:ARG:C	2.40	0.46
1:D:78:ILE:N	3:D:2059:HOH:O	2.48	0.46
1:G:216:GLN:O	1:G:220:HIS:HD2	1.98	0.46
1:B:74:GLY:CA	1:B:107:ARG:HB2	2.46	0.46
1:C:56:ARG:HH11	1:C:56:ARG:HG2	1.81	0.46
1:C:239:LYS:HG2	1:D:24:ARG:HA	1.97	0.46
1:G:239:LYS:HB3	1:H:26:LEU:HD23	1.97	0.46
1:A:148:LEU:O	1:A:151:ILE:HG12	2.15	0.46
1:D:52:LYS:HB3	1:D:56:ARG:HH12	1.81	0.46
1:E:321:GLU:HA	1:E:344:CYS:O	2.16	0.46
1:E:335:LYS:HB3	1:E:338:VAL:CG1	2.45	0.46
1:G:359:ALA:HA	1:G:362:ARG:NE	2.30	0.46
1:A:207:THR:HG22	1:A:253:LYS:HD3	1.96	0.46
1:B:59:ILE:HD13	1:B:243:HIS:CE1	2.51	0.46
1:B:119:TRP:CZ3	1:B:340:ILE:HD11	2.50	0.46
1:E:119:TRP:CZ3	1:E:340:ILE:HD11	2.51	0.46
1:E:308:ASN:ND2	1:E:364:ARG:HD3	2.30	0.46
1:G:239:LYS:HE2	1:H:26:LEU:HD23	1.97	0.46
1:H:32:ALA:HB1	1:H:36:LEU:HD23	1.96	0.46
1:E:127:ASP:HB3	1:E:129:ASN:ND2	2.31	0.46
1:E:321:GLU:HB3	1:E:346:GLY:N	2.30	0.46
1:F:67:ASP:OD2	1:F:365:ARG:CG	2.63	0.46
1:H:164:SER:OG	1:H:165:PRO:HD3	2.16	0.46
1:A:52:LYS:HD2	1:A:52:LYS:N	2.30	0.46
1:D:266:LYS:HD3	3:D:2160:HOH:O	2.14	0.46
1:E:94:LEU:HD13	1:E:94:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PHE:CD2	1:B:343:ALA:HB1	2.51	0.46
1:D:52:LYS:HB3	1:D:56:ARG:NH1	2.31	0.46
1:E:237:THR:HG22	1:F:26:LEU:HB2	1.97	0.46
1:B:201:LYS:HD2	1:B:249:ARG:HG2	1.97	0.46
1:B:93:LYS:O	1:B:96:ASP:HB2	2.15	0.46
1:C:164:SER:N	1:C:165:PRO:CD	2.79	0.46
1:H:110:LEU:HD11	1:H:145:PHE:CZ	2.50	0.46
1:B:44:THR:OG1	1:B:150:ASN:ND2	2.49	0.46
1:H:175:GLY:HA3	1:H:196:PHE:HE1	1.81	0.46
1:A:257:TYR:CG	1:A:295:VAL:HG13	2.50	0.45
1:D:146:VAL:O	1:D:150:ASN:HB2	2.16	0.45
1:F:266:LYS:HE2	3:F:2133:HOH:O	2.16	0.45
1:G:205:ASP:OD2	1:H:252:LYS:NZ	2.38	0.45
1:H:249:ARG:HD3	1:H:249:ARG:C	2.41	0.45
1:D:127:ASP:O	1:D:128:VAL:HG22	2.17	0.45
1:G:78:ILE:CD1	3:G:2023:HOH:O	2.64	0.45
1:G:180:ARG:HG3	1:G:180:ARG:HH11	1.81	0.45
1:G:207:THR:HG22	1:G:209:ASN:H	1.81	0.45
1:C:55:ARG:O	1:C:59:ILE:HG13	2.16	0.45
1:G:93:LYS:HD3	1:G:94:LEU:H	1.72	0.45
1:C:294:LYS:O	1:C:298:VAL:HG23	2.17	0.45
1:E:93:LYS:HD3	1:E:93:LYS:C	2.41	0.45
1:G:324:GLN:NE2	1:G:338:VAL:HB	2.32	0.45
1:H:110:LEU:HD13	1:H:141:ALA:HB1	1.97	0.45
1:H:324:GLN:NE2	1:H:334:LEU:HB3	2.31	0.45
1:C:60:ASP:OD1	1:C:65:LYS:CE	2.64	0.45
1:D:175:GLY:O	1:D:198:VAL:HA	2.17	0.45
1:F:135:ASN:O	1:F:139:GLN:HG3	2.17	0.45
1:F:280:TYR:CE1	1:F:313:VAL:HG22	2.51	0.45
1:H:34:PRO:HA	1:H:167:TYR:CD2	2.52	0.45
1:H:198:VAL:O	1:H:244:CYS:HA	2.16	0.45
1:H:208:LEU:N	1:H:208:LEU:HD12	2.31	0.45
1:C:297:ASP:HB2	3:C:2128:HOH:O	2.17	0.45
1:D:289:PHE:HA	3:D:2167:HOH:O	2.16	0.45
1:E:148:LEU:O	1:E:151:ILE:HG12	2.16	0.45
1:G:239:LYS:HE2	1:H:26:LEU:CD2	2.47	0.45
1:G:281:SER:CA	1:G:285:SER:HB2	2.45	0.45
1:B:127:ASP:O	1:B:128:VAL:HG22	2.17	0.45
1:C:189:GLU:HB3	1:C:224:PHE:CE2	2.52	0.45
1:E:39:VAL:HG21	1:G:30:PRO:CG	2.45	0.45
1:E:78:ILE:CD1	3:E:2012:HOH:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LYS:HB3	1:F:26:LEU:HD23	1.99	0.45
1:F:67:ASP:OD2	1:F:365:ARG:HG2	2.17	0.45
1:F:177:ILE:HG13	1:F:200:PHE:CE2	2.52	0.45
1:G:277:MET:HG3	1:G:312:GLY:C	2.41	0.45
1:H:34:PRO:HG3	1:H:167:TYR:CE1	2.50	0.45
1:H:74:GLY:HA3	1:H:107:ARG:HB2	1.98	0.45
1:B:139:GLN:NE2	3:B:2072:HOH:O	2.46	0.45
1:B:286:ASN:HD22	1:B:286:ASN:HA	1.53	0.45
1:G:352:ASP:O	1:G:356:LYS:HG3	2.17	0.45
1:A:292:GLN:N	1:A:293:PRO:HD2	2.32	0.45
1:B:355:ARG:HG3	1:B:355:ARG:HH11	1.80	0.45
1:C:335:LYS:HE3	1:C:335:LYS:HA	1.98	0.45
1:C:359:ALA:CA	1:C:362:ARG:HH21	2.30	0.45
1:D:288:ASP:OD1	1:D:290:ARG:HB2	2.17	0.45
1:G:40:GLN:HG3	1:G:41:ILE:HG12	1.99	0.45
1:H:202:ASN:HB2	1:H:207:THR:O	2.16	0.45
1:F:34:PRO:O	1:F:38:GLN:HG3	2.18	0.44
1:F:364:ARG:O	1:F:368:ASN:ND2	2.50	0.44
1:B:43:ALA:CB	1:B:171:LEU:HD21	2.47	0.44
1:C:327:PRO:HG3	1:C:333:GLY:O	2.18	0.44
1:E:28:TYR:HA	1:F:235:ILE:O	2.17	0.44
1:H:107:ARG:NH2	3:H:2024:HOH:O	2.48	0.44
1:H:174:PHE:CZ	1:H:176:ALA:HB2	2.52	0.44
1:H:175:GLY:O	1:H:198:VAL:HA	2.18	0.44
1:B:202:ASN:HB2	1:B:207:THR:O	2.17	0.44
1:C:26:LEU:HD23	1:C:26:LEU:O	2.17	0.44
1:G:126:PRO:HB3	1:G:137:GLY:HA2	1.99	0.44
1:G:191:ALA:HA	1:G:194:LEU:HD12	1.99	0.44
1:G:288:ASP:HB3	1:G:291:ASN:ND2	2.32	0.44
1:H:34:PRO:HD2	1:H:229:LYS:O	2.17	0.44
1:C:359:ALA:HA	1:C:362:ARG:NE	2.27	0.44
1:C:364:ARG:O	1:C:368:ASN:ND2	2.50	0.44
1:D:79:HIS:HD2	3:D:2032:HOH:O	2.00	0.44
1:D:198:VAL:O	1:D:244:CYS:HA	2.17	0.44
1:D:205:ASP:O	1:D:253:LYS:HB3	2.17	0.44
1:F:357:LEU:O	1:F:361:VAL:HG23	2.17	0.44
1:G:51:ALA:O	1:G:55:ARG:HG3	2.16	0.44
1:A:72:ILE:HG22	1:A:107:ARG:HG3	1.99	0.44
1:B:198:VAL:O	1:B:244:CYS:HA	2.17	0.44
1:C:279:ASP:HA	1:C:314:MET:HB3	1.99	0.44
1:E:307:GLU:OE2	1:E:309:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ASP:CG	1:F:365:ARG:HH11	2.25	0.44
1:D:255:THR:HG23	3:D:2153:HOH:O	2.18	0.44
1:E:240:GLY:O	1:F:24:ARG:HD3	2.18	0.44
1:E:348:GLU:CD	1:E:348:GLU:N	2.55	0.44
1:G:90:ARG:O	1:G:93:LYS:HG3	2.18	0.44
1:B:174:PHE:CE1	1:B:176:ALA:HB2	2.52	0.44
1:E:248:LEU:HB3	1:E:256:ASN:OD1	2.18	0.44
1:E:289:PHE:CD1	1:E:289:PHE:C	2.96	0.44
1:G:117:VAL:HG11	1:H:220:HIS:CD2	2.53	0.44
1:A:73:VAL:O	1:A:106:MET:HA	2.18	0.44
1:A:96:ASP:O	1:A:99:LYS:HG2	2.17	0.44
1:C:74:GLY:CA	1:C:107:ARG:HB2	2.48	0.44
1:C:201:LYS:HD2	1:C:249:ARG:HG2	2.00	0.44
1:G:266:LYS:HD2	1:G:309:ALA:CB	2.48	0.44
1:H:306:GLY:HA2	1:H:367:VAL:HG21	2.00	0.44
1:A:319:ILE:HB	1:A:337:GLY:HA3	2.00	0.44
1:B:223:HIS:CE1	1:B:237:THR:HG23	2.52	0.44
1:B:255:THR:HG22	1:B:284:ASN:HA	1.99	0.44
1:F:166:GLN:O	1:F:229:LYS:HE2	2.18	0.44
1:G:101:ASP:HA	1:G:365:ARG:HH22	1.83	0.44
1:H:296:ASN:CG	1:H:353:VAL:HG13	2.43	0.44
1:C:73:VAL:HG23	1:C:315:ILE:HB	2.00	0.43
1:C:110:LEU:CD1	1:C:141:ALA:HB1	2.48	0.43
1:D:269:LEU:HD11	1:D:276:LEU:HD21	1.99	0.43
1:E:205:ASP:HA	1:E:252:LYS:HB2	1.99	0.43
1:G:67:ASP:OD2	1:G:365:ARG:HD3	2.18	0.43
1:G:93:LYS:CD	1:G:94:LEU:N	2.66	0.43
1:G:119:TRP:NE1	1:G:128:VAL:HG12	2.32	0.43
1:G:252:LYS:NZ	1:H:207:THR:HG21	2.33	0.43
1:H:90:ARG:HA	1:H:93:LYS:HE3	2.00	0.43
1:H:257:TYR:CG	1:H:295:VAL:HG13	2.53	0.43
1:F:266:LYS:HD2	1:F:309:ALA:CB	2.47	0.43
1:A:37:LEU:CD1	1:A:142:ARG:HD3	2.49	0.43
1:A:129:ASN:ND2	1:A:131:THR:CG2	2.82	0.43
1:B:141:ALA:O	1:B:144:LEU:HB3	2.18	0.43
1:C:290:ARG:HH11	1:C:290:ARG:HG2	1.82	0.43
1:D:266:LYS:HE3	1:D:309:ALA:HB2	2.00	0.43
1:F:355:ARG:HG3	1:F:355:ARG:HH11	1.83	0.43
1:C:28:TYR:HA	1:D:235:ILE:O	2.18	0.43
1:C:78:ILE:N	1:C:78:ILE:HD12	2.34	0.43
1:C:363:GLN:CA	1:C:363:GLN:HE21	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ASP:HB2	1:D:129:ASN:HD21	1.83	0.43
1:D:159:MET:HA	1:D:159:MET:HE2	2.01	0.43
1:E:295:VAL:O	1:E:299:VAL:HG23	2.17	0.43
1:F:202:ASN:HB3	1:F:208:LEU:HD12	1.99	0.43
1:F:296:ASN:CG	1:F:353:VAL:HG13	2.44	0.43
1:G:110:LEU:O	1:G:121:GLY:HA3	2.18	0.43
1:G:202:ASN:C	1:G:202:ASN:ND2	2.74	0.43
1:G:242:GLU:HG2	1:G:243:HIS:CD2	2.53	0.43
1:H:296:ASN:ND2	1:H:353:VAL:HG13	2.33	0.43
1:A:110:LEU:HD23	3:A:2068:HOH:O	2.17	0.43
1:C:205:ASP:HB3	3:C:2095:HOH:O	2.17	0.43
1:H:168:LEU:HD22	1:H:168:LEU:N	2.34	0.43
1:A:110:LEU:HD21	1:A:145:PHE:CZ	2.53	0.43
1:E:288:ASP:HB3	1:E:291:ASN:HD21	1.81	0.43
1:G:148:LEU:O	1:G:151:ILE:HG12	2.19	0.43
1:G:239:LYS:HB3	1:G:239:LYS:HE2	1.72	0.43
1:G:326:ILE:HG23	1:G:340:ILE:HD11	2.00	0.43
1:A:277:MET:HA	1:A:312:GLY:O	2.18	0.43
1:C:263:ALA:HB2	3:C:2120:HOH:O	2.18	0.43
1:H:277:MET:HA	1:H:312:GLY:O	2.18	0.43
1:A:247:ILE:HG12	1:A:277:MET:HB3	2.00	0.43
1:C:185:GLN:O	1:C:189:GLU:HG3	2.19	0.43
1:C:326:ILE:HG13	1:C:326:ILE:O	2.18	0.43
1:D:148:LEU:O	1:D:151:ILE:HG12	2.18	0.43
1:D:161:ASP:HB3	1:D:164:SER:OG	2.17	0.43
1:E:239:LYS:HG2	1:F:24:ARG:CA	2.48	0.43
1:H:208:LEU:N	1:H:208:LEU:CD1	2.82	0.43
1:H:355:ARG:O	1:H:358:ALA:HB3	2.18	0.43
1:A:55:ARG:O	1:A:59:ILE:HG13	2.18	0.43
1:A:108:ALA:O	1:A:110:LEU:HD22	2.18	0.43
1:B:161:ASP:HB3	1:B:164:SER:OG	2.19	0.43
1:C:148:LEU:O	1:C:151:ILE:HG12	2.19	0.43
1:D:59:ILE:O	1:D:63:THR:HG23	2.19	0.43
1:E:298:VAL:O	1:E:301:GLU:CG	2.66	0.43
1:G:248:LEU:HD22	1:G:248:LEU:H	1.84	0.43
1:D:303:ILE:O	1:D:364:ARG:HB2	2.18	0.43
1:E:41:ILE:O	1:E:41:ILE:HG22	2.19	0.43
1:G:77:SER:HB3	1:G:112:LYS:CD	2.45	0.43
1:A:175:GLY:O	1:A:198:VAL:HA	2.19	0.42
1:B:277:MET:HA	1:B:312:GLY:O	2.19	0.42
1:E:128:VAL:HG12	1:E:128:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ARG:O	1:E:283:GLY:HA3	2.19	0.42
1:H:210:VAL:HG13	3:H:2091:HOH:O	2.17	0.42
1:C:221:SER:HB2	1:C:238:THR:O	2.19	0.42
1:G:239:LYS:HG2	1:H:24:ARG:HA	2.01	0.42
1:G:298:VAL:O	1:G:302:GLN:HG3	2.19	0.42
1:B:72:ILE:HG12	1:B:277:MET:HE1	2.00	0.42
1:C:95:SER:O	1:C:99:LYS:N	2.52	0.42
1:C:290:ARG:HG2	1:C:290:ARG:NH1	2.34	0.42
1:D:252:LYS:HE2	3:D:2120:HOH:O	2.20	0.42
1:E:293:PRO:O	1:E:296:ASN:HB3	2.20	0.42
1:F:351:GLU:O	1:F:355:ARG:HD3	2.19	0.42
1:G:67:ASP:OD2	1:G:365:ARG:CG	2.67	0.42
1:H:43:ALA:CB	1:H:48:LEU:HD21	2.50	0.42
1:H:202:ASN:C	1:H:202:ASN:HD22	2.26	0.42
1:A:145:PHE:HB3	1:A:171:LEU:HD13	2.01	0.42
1:A:232:VAL:HG12	1:B:232:VAL:HG12	2.00	0.42
1:B:291:ASN:O	1:B:295:VAL:HG23	2.19	0.42
1:D:292:GLN:N	1:D:293:PRO:HD2	2.34	0.42
1:F:164:SER:N	1:F:165:PRO:CD	2.82	0.42
1:G:127:ASP:C	1:G:128:VAL:HG22	2.45	0.42
1:H:135:ASN:HB2	3:H:2061:HOH:O	2.20	0.42
1:B:114:ARG:HA	1:B:114:ARG:HD3	1.82	0.42
1:B:127:ASP:C	1:B:128:VAL:HG22	2.45	0.42
1:F:321:GLU:HB3	1:F:346:GLY:H	1.84	0.42
1:G:189:GLU:HB3	1:G:224:PHE:CD2	2.55	0.42
1:G:317:SER:HB2	1:G:350:THR:OG1	2.19	0.42
1:D:348:GLU:CD	1:D:348:GLU:N	2.76	0.42
1:E:296:ASN:O	1:E:297:ASP:C	2.62	0.42
1:F:142:ARG:O	1:F:146:VAL:HG23	2.19	0.42
1:G:74:GLY:CA	1:G:107:ARG:HB2	2.49	0.42
1:H:205:ASP:HA	1:H:252:LYS:HB2	2.01	0.42
1:A:75:PRO:HB2	1:A:78:ILE:HD12	2.02	0.42
1:E:24:ARG:HD2	1:F:194:LEU:O	2.20	0.42
1:E:41:ILE:O	1:E:142:ARG:NH2	2.53	0.42
1:G:317:SER:HA	1:G:344:CYS:HB3	2.02	0.42
1:H:74:GLY:CA	1:H:107:ARG:HB2	2.49	0.42
1:C:249:ARG:O	1:C:283:GLY:HA3	2.20	0.42
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.89	0.42
1:H:79:HIS:CD2	1:H:340:ILE:HG12	2.55	0.42
1:A:216:GLN:HA	1:A:216:GLN:NE2	2.27	0.42
1:E:34:PRO:HG3	1:E:167:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:GLU:O	1:F:267:ALA:HB3	2.19	0.42
1:A:190:LEU:O	1:A:194:LEU:HG	2.20	0.41
1:A:289:PHE:CD2	1:A:343:ALA:HB1	2.55	0.41
1:C:353:VAL:O	1:C:357:LEU:HB2	2.19	0.41
1:D:206:GLY:CA	1:D:251:GLY:HA3	2.50	0.41
1:D:289:PHE:CE1	1:D:290:ARG:HG3	2.54	0.41
1:B:34:PRO:O	1:B:38:GLN:HG3	2.21	0.41
1:C:95:SER:O	1:C:99:LYS:HB3	2.19	0.41
1:C:115:THR:O	1:D:188:ARG:NH1	2.52	0.41
1:C:335:LYS:HB2	1:C:338:VAL:HG22	2.01	0.41
1:F:101:ASP:OD1	1:F:365:ARG:NH2	2.52	0.41
1:A:37:LEU:HD21	1:A:139:GLN:HG2	2.02	0.41
1:E:79:HIS:CD2	3:E:2097:HOH:O	2.73	0.41
1:E:86:GLU:HA	1:E:89:LEU:HG	2.02	0.41
1:E:198:VAL:O	1:E:244:CYS:HA	2.20	0.41
1:F:201:LYS:NZ	2:F:500:PEP:O2	2.53	0.41
1:D:119:TRP:CZ2	1:D:128:VAL:HG12	2.55	0.41
1:D:216:GLN:NE2	3:D:2129:HOH:O	2.52	0.41
1:E:129:ASN:OD1	1:E:131:THR:CG2	2.68	0.41
1:F:247:ILE:HA	1:F:277:MET:O	2.21	0.41
1:C:202:ASN:HB2	1:C:207:THR:O	2.20	0.41
1:H:333:GLY:H	1:H:334:LEU:HD23	1.84	0.41
1:B:43:ALA:CB	1:B:48:LEU:CD2	2.98	0.41
1:D:110:LEU:HD11	1:D:145:PHE:CZ	2.55	0.41
1:E:201:LYS:HB3	1:E:249:ARG:HG2	2.03	0.41
1:C:277:MET:HG3	1:C:312:GLY:C	2.45	0.41
1:D:85:GLN:O	1:D:89:LEU:CD2	2.69	0.41
1:D:127:ASP:HB2	1:D:129:ASN:ND2	2.36	0.41
1:G:327:PRO:O	1:G:332:ALA:HB2	2.21	0.41
1:A:67:ASP:OD1	1:A:365:ARG:NH1	2.54	0.41
1:B:280:TYR:O	1:B:292:GLN:HG2	2.20	0.41
1:C:34:PRO:HA	1:C:167:TYR:CD2	2.55	0.41
1:C:324:GLN:NE2	1:C:338:VAL:CG2	2.84	0.41
1:D:96:ASP:O	1:D:99:LYS:HD2	2.20	0.41
1:G:43:ALA:CB	1:G:48:LEU:HD21	2.51	0.41
1:A:78:ILE:CD1	3:A:2038:HOH:O	2.68	0.41
1:C:89:LEU:HD12	1:C:151:ILE:CD1	2.51	0.41
1:C:128:VAL:O	1:C:128:VAL:HG23	2.20	0.41
1:C:198:VAL:O	1:C:244:CYS:HA	2.21	0.41
1:D:150:ASN:HB3	3:D:2087:HOH:O	2.21	0.41
1:E:93:LYS:HD3	1:E:94:LEU:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ALA:O	1:E:110:LEU:HD22	2.21	0.41
1:F:146:VAL:O	1:F:150:ASN:HB2	2.21	0.41
1:G:26:LEU:HB2	1:H:237:THR:O	2.21	0.41
1:G:109:TYR:CE2	1:G:158:GLU:HB2	2.56	0.41
1:G:289:PHE:CZ	1:G:321:GLU:HB2	2.56	0.41
1:H:72:ILE:HG12	1:H:277:MET:HE1	2.02	0.41
1:H:119:TRP:CZ2	1:H:128:VAL:HG12	2.56	0.41
1:H:177:ILE:O	1:H:201:LYS:HG3	2.21	0.41
1:H:334:LEU:HD22	1:H:340:ILE:CG2	2.51	0.41
1:C:48:LEU:N	1:C:48:LEU:HD22	2.36	0.41
1:F:201:LYS:HD3	1:F:247:ILE:HB	2.03	0.41
1:G:189:GLU:HB3	1:G:224:PHE:CE2	2.56	0.41
1:H:79:HIS:CE1	1:H:334:LEU:CD1	3.02	0.41
1:D:43:ALA:CB	1:D:171:LEU:HD21	2.51	0.40
1:D:306:GLY:HA2	1:D:367:VAL:HG21	2.02	0.40
1:E:164:SER:N	1:E:165:PRO:CD	2.84	0.40
1:E:238:THR:HG22	1:F:25:ILE:HD13	2.03	0.40
1:G:124:ASN:O	1:G:132:PHE:HA	2.22	0.40
1:G:336:TYR:CD1	1:G:336:TYR:C	2.99	0.40
1:H:355:ARG:HD2	1:H:355:ARG:HA	1.89	0.40
1:C:310:ILE:O	1:C:364:ARG:NH2	2.54	0.40
1:E:335:LYS:HB3	1:E:338:VAL:HG11	2.04	0.40
1:G:99:LYS:HE3	1:G:99:LYS:HB2	1.95	0.40
1:A:127:ASP:O	1:A:128:VAL:C	2.63	0.40
1:A:288:ASP:OD2	1:A:290:ARG:HB2	2.21	0.40
1:C:93:LYS:HG3	1:C:94:LEU:N	2.37	0.40
1:C:331:LYS:C	1:C:334:LEU:HD21	2.46	0.40
1:D:127:ASP:C	1:D:128:VAL:HG22	2.46	0.40
1:E:86:GLU:O	1:E:90:ARG:HG3	2.21	0.40
1:G:321:GLU:HA	1:G:344:CYS:O	2.20	0.40
1:H:37:LEU:HD22	1:H:37:LEU:HA	1.94	0.40
1:H:110:LEU:HB3	1:H:123:ILE:HG13	2.02	0.40
1:H:323:ASN:N	1:H:323:ASN:OD1	2.54	0.40
1:A:336:TYR:O	1:A:338:VAL:N	2.49	0.40
1:B:164:SER:N	1:B:165:PRO:CD	2.85	0.40
1:E:242:GLU:HG2	1:E:243:HIS:CD2	2.57	0.40
1:G:119:TRP:CZ2	1:G:128:VAL:HG12	2.57	0.40
1:G:334:LEU:HD11	1:G:340:ILE:CD1	2.50	0.40
1:G:351:GLU:HG2	1:G:355:ARG:NH1	2.37	0.40
1:H:90:ARG:CA	1:H:93:LYS:HE3	2.52	0.40
1:H:292:GLN:N	1:H:293:PRO:HD2	2.36	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	335/370 (90%)	317 (95%)	16 (5%)	2 (1%)	21	13
1	B	332/370 (90%)	322 (97%)	10 (3%)	0	100	100
1	C	346/370 (94%)	328 (95%)	16 (5%)	2 (1%)	21	13
1	D	338/370 (91%)	326 (96%)	12 (4%)	0	100	100
1	E	331/370 (90%)	317 (96%)	13 (4%)	1 (0%)	36	29
1	F	344/370 (93%)	328 (95%)	16 (5%)	0	100	100
1	G	340/370 (92%)	310 (91%)	25 (7%)	5 (2%)	8	2
1	H	337/370 (91%)	321 (95%)	12 (4%)	4 (1%)	10	4
All	All	2703/2960 (91%)	2569 (95%)	120 (4%)	14 (0%)	24	16

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TYR
1	C	336	TYR
1	G	130	ASN
1	G	327	PRO
1	G	332	ALA
1	G	367	VAL
1	H	325	GLY
1	H	324	GLN
1	H	334	LEU
1	C	270	PRO
1	G	128	VAL
1	H	333	GLY
1	A	337	GLY
1	E	128	VAL

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	276/298 (93%)	260 (94%)	16 (6%)	18	10
1	B	274/298 (92%)	259 (94%)	15 (6%)	19	11
1	C	281/298 (94%)	271 (96%)	10 (4%)	31	23
1	D	277/298 (93%)	263 (95%)	14 (5%)	21	13
1	E	273/298 (92%)	257 (94%)	16 (6%)	18	10
1	F	279/298 (94%)	262 (94%)	17 (6%)	17	9
1	G	277/298 (93%)	262 (95%)	15 (5%)	20	12
1	H	275/298 (92%)	260 (94%)	15 (6%)	19	11
All	All	2212/2384 (93%)	2094 (95%)	118 (5%)	20	12

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	53	ARG
1	A	73	VAL
1	A	93	LYS
1	A	96	ASP
1	A	110	LEU
1	A	129	ASN
1	A	181	THR
1	A	202	ASN
1	A	208	LEU
1	A	216	GLN
1	A	249	ARG
1	A	349	THR
1	A	357	LEU
1	A	363	GLN
1	A	366	GLU
1	B	26	LEU
1	B	37	LEU
1	B	52	LYS

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Mol	Chain	Res	Type
1	B	56	ARG
1	B	110	LEU
1	B	148	LEU
1	B	202	ASN
1	B	249	ARG
1	B	253	LYS
1	B	260	LYS
1	B	281	SER
1	B	286	ASN
1	B	338	VAL
1	B	355	ARG
1	B	363	GLN
1	C	37	LEU
1	C	94	LEU
1	C	208	LEU
1	C	249	ARG
1	C	253	LYS
1	C	331	LYS
1	C	348	GLU
1	C	357	LEU
1	C	363	GLN
1	C	370	LYS
1	D	94	LEU
1	D	114	ARG
1	D	129	ASN
1	D	202	ASN
1	D	208	LEU
1	D	216	GLN
1	D	248	LEU
1	D	249	ARG
1	D	253	LYS
1	D	255	THR
1	D	290	ARG
1	D	357	LEU
1	D	363	GLN
1	D	369	LYS
1	E	89	LEU
1	E	93	LYS
1	E	110	LEU
1	E	168	LEU
1	E	202	ASN
1	E	216	GLN

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Mol	Chain	Res	Type
1	E	249	ARG
1	E	253	LYS
1	E	276	LEU
1	E	290	ARG
1	E	301	GLU
1	E	348	GLU
1	E	355	ARG
1	E	357	LEU
1	E	363	GLN
1	E	366	GLU
1	F	37	LEU
1	F	48	LEU
1	F	78	ILE
1	F	89	LEU
1	F	93	LYS
1	F	110	LEU
1	F	128	VAL
1	F	148	LEU
1	F	168	LEU
1	F	202	ASN
1	F	209	ASN
1	F	276	LEU
1	F	301	GLU
1	F	313	VAL
1	F	331	LYS
1	F	355	ARG
1	F	363	GLN
1	G	37	LEU
1	G	89	LEU
1	G	93	LYS
1	G	98	LEU
1	G	110	LEU
1	G	115	THR
1	G	148	LEU
1	G	202	ASN
1	G	204	THR
1	G	216	GLN
1	G	249	ARG
1	G	255	THR
1	G	321	GLU
1	G	355	ARG
1	G	357	LEU

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Mol	Chain	Res	Type
1	H	26	LEU
1	H	37	LEU
1	H	78	ILE
1	H	86	GLU
1	H	89	LEU
1	H	148	LEU
1	H	168	LEU
1	H	202	ASN
1	H	208	LEU
1	H	249	ARG
1	H	290	ARG
1	H	334	LEU
1	H	338	VAL
1	H	355	ARG
1	H	363	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	40	GLN
1	A	129	ASN
1	A	130	ASN
1	A	139	GLN
1	A	143	GLN
1	A	216	GLN
1	A	220	HIS
1	A	291	ASN
1	A	308	ASN
1	A	368	ASN
1	B	79	HIS
1	B	85	GLN
1	B	130	ASN
1	B	143	GLN
1	B	147	ASN
1	B	150	ASN
1	B	166	GLN
1	B	286	ASN
1	B	308	ASN
1	B	368	ASN
1	C	38	GLN
1	C	40	GLN

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Mol	Chain	Res	Type
1	C	79	HIS
1	C	130	ASN
1	C	139	GLN
1	C	150	ASN
1	C	220	HIS
1	C	305	ASN
1	C	308	ASN
1	C	320	ASN
1	C	363	GLN
1	C	368	ASN
1	D	38	GLN
1	D	40	GLN
1	D	79	HIS
1	D	85	GLN
1	D	129	ASN
1	D	139	GLN
1	D	147	ASN
1	D	216	GLN
1	D	220	HIS
1	D	268	GLN
1	D	308	ASN
1	D	363	GLN
1	D	368	ASN
1	E	40	GLN
1	E	130	ASN
1	E	139	GLN
1	E	143	GLN
1	E	147	ASN
1	E	150	ASN
1	E	216	GLN
1	E	220	HIS
1	E	286	ASN
1	E	292	GLN
1	E	308	ASN
1	E	368	ASN
1	F	40	GLN
1	F	130	ASN
1	F	150	ASN
1	F	209	ASN
1	F	220	HIS
1	F	268	GLN
1	F	286	ASN

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Mol	Chain	Res	Type
1	F	363	GLN
1	G	130	ASN
1	G	166	GLN
1	G	216	GLN
1	G	220	HIS
1	G	286	ASN
1	G	291	ASN
1	G	318	ASN
1	G	363	GLN
1	G	368	ASN
1	H	79	HIS
1	H	130	ASN
1	H	220	HIS
1	H	282	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	F	500	-	9,9,9	2.81	2 (22%)	11,13,13	2.00	2 (18%)
2	PEP	D	500	-	9,9,9	2.96	3 (33%)	11,13,13	2.03	2 (18%)
2	PEP	B	500	-	9,9,9	2.96	3 (33%)	11,13,13	2.03	2 (18%)
2	PEP	A	500	-	9,9,9	2.73	2 (22%)	11,13,13	1.98	2 (18%)
2	PEP	H	500	-	9,9,9	2.92	3 (33%)	11,13,13	2.03	2 (18%)
2	PEP	E	500	-	9,9,9	3.08	3 (33%)	11,13,13	2.12	2 (18%)
2	PEP	G	500	-	9,9,9	3.22	3 (33%)	11,13,13	2.17	2 (18%)
2	PEP	C	500	-	9,9,9	2.90	2 (22%)	11,13,13	2.05	3 (27%)

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	F	500	-	-	0/9/9/9	-
2	PEP	D	500	-	-	0/9/9/9	-
2	PEP	B	500	-	-	0/9/9/9	-
2	PEP	A	500	-	-	0/9/9/9	-
2	PEP	H	500	-	-	0/9/9/9	-
2	PEP	E	500	-	-	0/9/9/9	-
2	PEP	G	500	-	-	0/9/9/9	-
2	PEP	C	500	-	-	0/9/9/9	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	PEP	O2-C2	8.36	1.62	1.39
2	E	500	PEP	O2-C2	8.02	1.61	1.39
2	H	500	PEP	O2-C2	7.73	1.60	1.39
2	D	500	PEP	O2-C2	7.57	1.60	1.39
2	B	500	PEP	O2-C2	7.55	1.60	1.39
2	C	500	PEP	O2-C2	7.54	1.60	1.39
2	F	500	PEP	O2-C2	7.37	1.59	1.39
2	A	500	PEP	O2-C2	7.01	1.58	1.39
2	G	500	PEP	C2-C1	2.68	1.52	1.49
2	C	500	PEP	C3-C2	2.64	1.38	1.31
2	B	500	PEP	C2-C1	2.63	1.51	1.49
2	A	500	PEP	C3-C2	2.61	1.38	1.31
2	E	500	PEP	C3-C2	2.57	1.38	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	PEP	C3-C2	2.57	1.38	1.31
2	F	500	PEP	C3-C2	2.57	1.38	1.31
2	B	500	PEP	C3-C2	2.56	1.38	1.31
2	D	500	PEP	C3-C2	2.55	1.38	1.31
2	H	500	PEP	C3-C2	2.54	1.38	1.31
2	D	500	PEP	C2-C1	2.51	1.51	1.49
2	E	500	PEP	C2-C1	2.18	1.51	1.49
2	H	500	PEP	O2'-C1	-2.05	1.25	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500	PEP	C3-C2-C1	-6.11	111.44	122.73
2	E	500	PEP	C3-C2-C1	-5.93	111.77	122.73
2	H	500	PEP	C3-C2-C1	-5.82	111.97	122.73
2	C	500	PEP	C3-C2-C1	-5.75	112.10	122.73
2	D	500	PEP	C3-C2-C1	-5.73	112.14	122.73
2	F	500	PEP	C3-C2-C1	-5.68	112.22	122.73
2	B	500	PEP	C3-C2-C1	-5.65	112.28	122.73
2	A	500	PEP	C3-C2-C1	-5.58	112.42	122.73
2	G	500	PEP	O2'-C1-C2	2.71	118.52	113.91
2	E	500	PEP	O2'-C1-C2	2.70	118.52	113.91
2	B	500	PEP	O2'-C1-C2	2.65	118.42	113.91
2	D	500	PEP	O2'-C1-C2	2.53	118.23	113.91
2	C	500	PEP	O2'-C1-C2	2.51	118.19	113.91
2	H	500	PEP	O2'-C1-C2	2.37	117.95	113.91
2	F	500	PEP	O2'-C1-C2	2.30	117.83	113.91
2	A	500	PEP	O2'-C1-C2	2.28	117.79	113.91
2	C	500	PEP	O1-C1-C2	-2.00	118.77	121.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	PEP	3	0
2	H	500	PEP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	339/370 (91%)	0.16	6 (1%) 67 71	17, 30, 43, 51	0
1	B	336/370 (90%)	0.14	7 (2%) 63 67	17, 29, 43, 51	0
1	C	348/370 (94%)	0.45	17 (4%) 35 37	19, 34, 49, 64	0
1	D	342/370 (92%)	0.04	6 (1%) 67 71	18, 27, 42, 57	0
1	E	335/370 (90%)	0.76	24 (7%) 21 23	21, 39, 51, 57	0
1	F	346/370 (93%)	0.13	8 (2%) 61 65	19, 30, 44, 56	0
1	G	342/370 (92%)	0.88	30 (8%) 15 16	23, 40, 52, 62	0
1	H	339/370 (91%)	0.27	8 (2%) 59 63	21, 32, 44, 66	0
All	All	2727/2960 (92%)	0.35	106 (3%) 43 46	17, 32, 48, 66	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	333	GLY	6.7
1	H	325	GLY	5.9
1	H	334	LEU	5.5
1	G	332	ALA	5.1
1	G	327	PRO	4.6
1	G	117	VAL	4.3
1	E	89	LEU	3.9
1	C	23	VAL	3.8
1	C	271	ALA	3.5
1	E	117	VAL	3.4
1	G	128	VAL	3.4
1	G	116	THR	3.4
1	F	208	LEU	3.3
1	F	28	TYR	3.1
1	G	340	ILE	3.1
1	A	128	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	23	VAL	3.1
1	D	369	LYS	3.0
1	E	128	VAL	3.0
1	E	110	LEU	3.0
1	F	331	LYS	3.0
1	H	89	LEU	2.9
1	E	23	VAL	2.9
1	E	28	TYR	2.9
1	E	116	THR	2.8
1	G	113	PRO	2.8
1	H	28	TYR	2.8
1	E	93	LYS	2.8
1	A	23	VAL	2.8
1	C	336	TYR	2.8
1	G	110	LEU	2.8
1	G	298	VAL	2.8
1	C	331	LYS	2.7
1	C	327	PRO	2.7
1	C	328	ALA	2.6
1	G	333	GLY	2.6
1	C	330	GLY	2.6
1	G	361	VAL	2.6
1	B	208	LEU	2.6
1	D	128	VAL	2.6
1	E	361	VAL	2.6
1	G	285	SER	2.6
1	G	286	ASN	2.6
1	H	23	VAL	2.6
1	B	119	TRP	2.5
1	E	285	SER	2.5
1	A	253	LYS	2.5
1	E	276	LEU	2.5
1	C	333	GLY	2.4
1	G	89	LEU	2.4
1	C	28	TYR	2.4
1	B	115	THR	2.4
1	B	23	VAL	2.4
1	F	23	VAL	2.4
1	C	89	LEU	2.4
1	E	153	LEU	2.4
1	D	28	TYR	2.4
1	G	115	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	347	TRP	2.4
1	G	119	TRP	2.4
1	G	276	LEU	2.3
1	B	28	TYR	2.3
1	F	368	ASN	2.3
1	D	367	VAL	2.3
1	E	115	THR	2.3
1	E	289	PHE	2.3
1	E	368	ASN	2.3
1	F	93	LYS	2.3
1	C	363	GLN	2.3
1	E	94	LEU	2.3
1	B	286	ASN	2.3
1	A	326	ILE	2.3
1	D	23	VAL	2.3
1	F	367	VAL	2.3
1	C	116	THR	2.3
1	E	151	ILE	2.2
1	G	368	ASN	2.2
1	H	368	ASN	2.2
1	G	300	CYS	2.2
1	C	337	GLY	2.2
1	F	328	ALA	2.2
1	E	286	ASN	2.1
1	G	326	ILE	2.1
1	E	352	ASP	2.1
1	E	367	VAL	2.1
1	C	276	LEU	2.1
1	B	369	LYS	2.1
1	E	335	LYS	2.1
1	D	332	ALA	2.1
1	H	216	GLN	2.1
1	C	56	ARG	2.1
1	G	28	TYR	2.1
1	G	101	ASP	2.1
1	E	287	LYS	2.1
1	G	120	LYS	2.1
1	G	325	GLY	2.1
1	G	271	ALA	2.1
1	G	358	ALA	2.1
1	E	319	ILE	2.0
1	G	287	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	2.0
1	C	208	LEU	2.0
1	G	208	LEU	2.0
1	C	332	ALA	2.0
1	A	93	LYS	2.0
1	G	73	VAL	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	PEP	H	500	10/10	0.93	0.10	26,34,38,40	0
2	PEP	B	500	10/10	0.95	0.09	25,29,30,34	0
2	PEP	D	500	10/10	0.95	0.08	27,31,33,33	0
2	PEP	F	500	10/10	0.95	0.08	20,25,28,28	0
2	PEP	G	500	10/10	0.95	0.09	38,43,44,46	0
2	PEP	A	500	10/10	0.95	0.08	20,25,29,32	0
2	PEP	E	500	10/10	0.96	0.08	33,37,43,43	0
2	PEP	C	500	10/10	0.96	0.07	24,28,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.