



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:49 AM UTC

PDB ID : 3K2Q / pdb_00003k2q
Title : Crystal structure of Pyrophosphate-dependent phosphofructokinase from *Marinobacter aquaeolei*, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET MqR88
Authors : Seetharaman, J.; Lew, S.; Wang, D.; Neely, H.; Janjua, K.; Cunningham, K.; Owens, L.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2009-09-30
Resolution : 2.50 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
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)

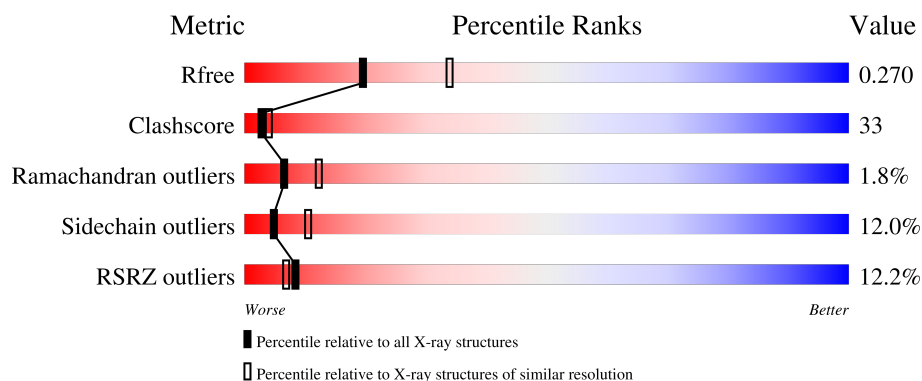
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	420	7% 48% 36% 8% 7%
1	B	420	12% 44% 41% 7% 7%
1	C	420	15% 45% 39% 8% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9397 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 Pyrophosphate-dependent phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3010	1909	519	566	16			
1	B	392	Total	C	N	O	S	0	0	0
			3010	1909	519	566	16			
1	C	392	Total	C	N	O	S	0	0	0
			3010	1909	519	566	16			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

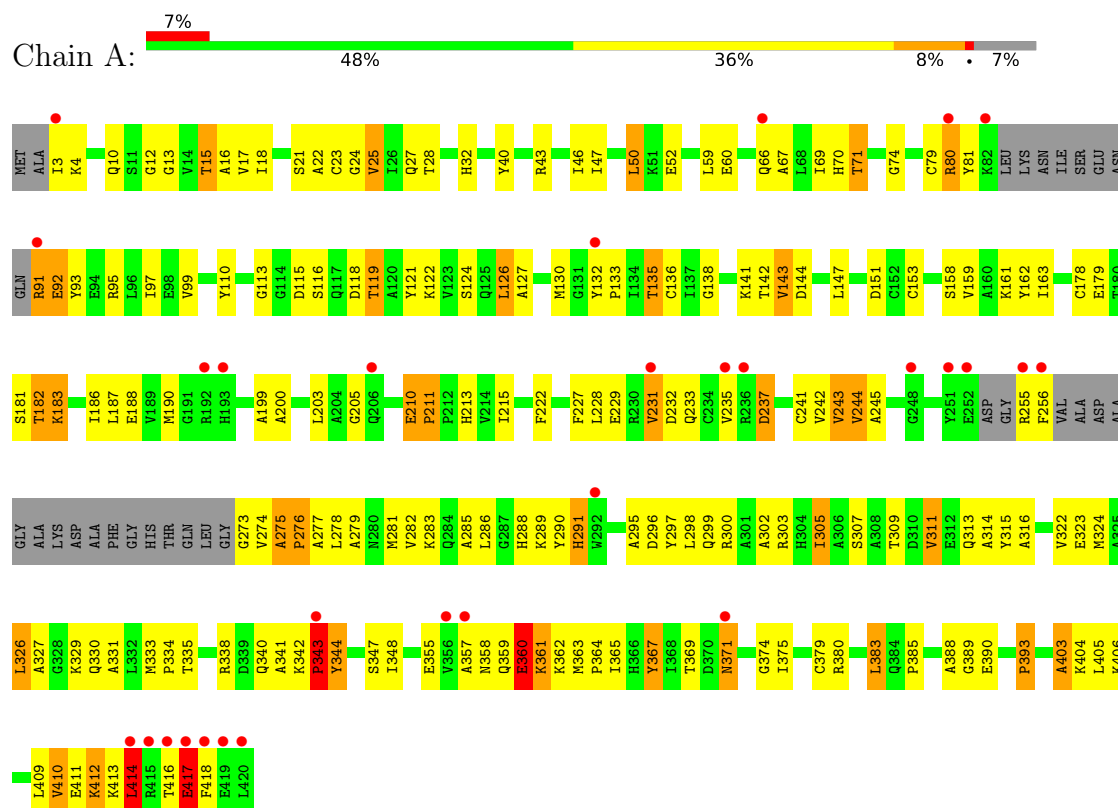
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	109	Total	O	0	0
			109	109		
3	C	119	Total	O	0	0
			119	119		

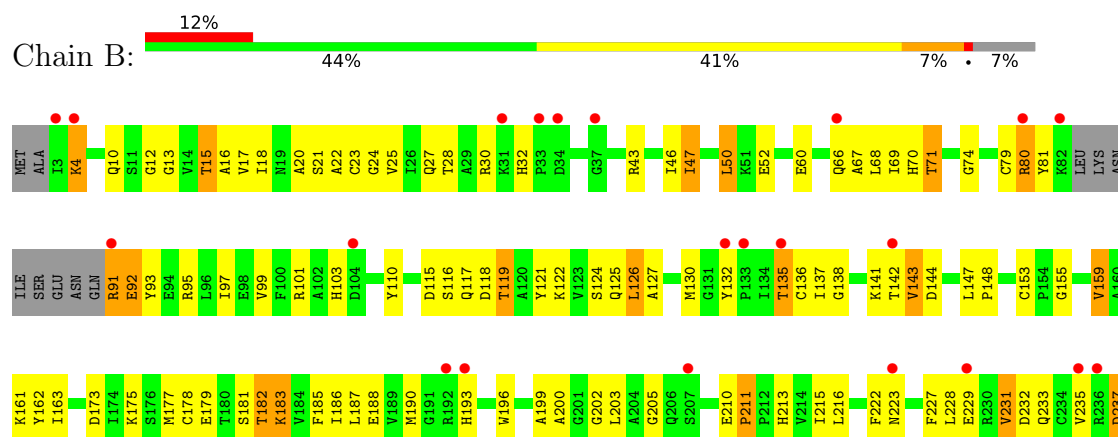
3 Residue-property plots [i](#)

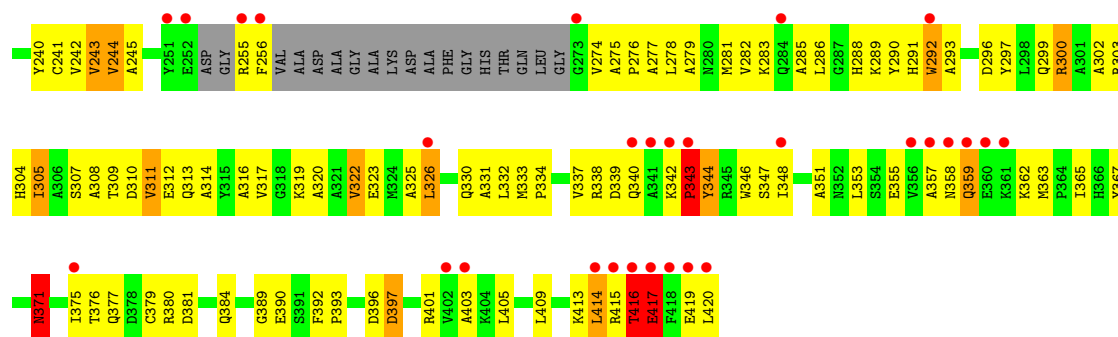
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyrophosphate-dependent phosphofructokinase

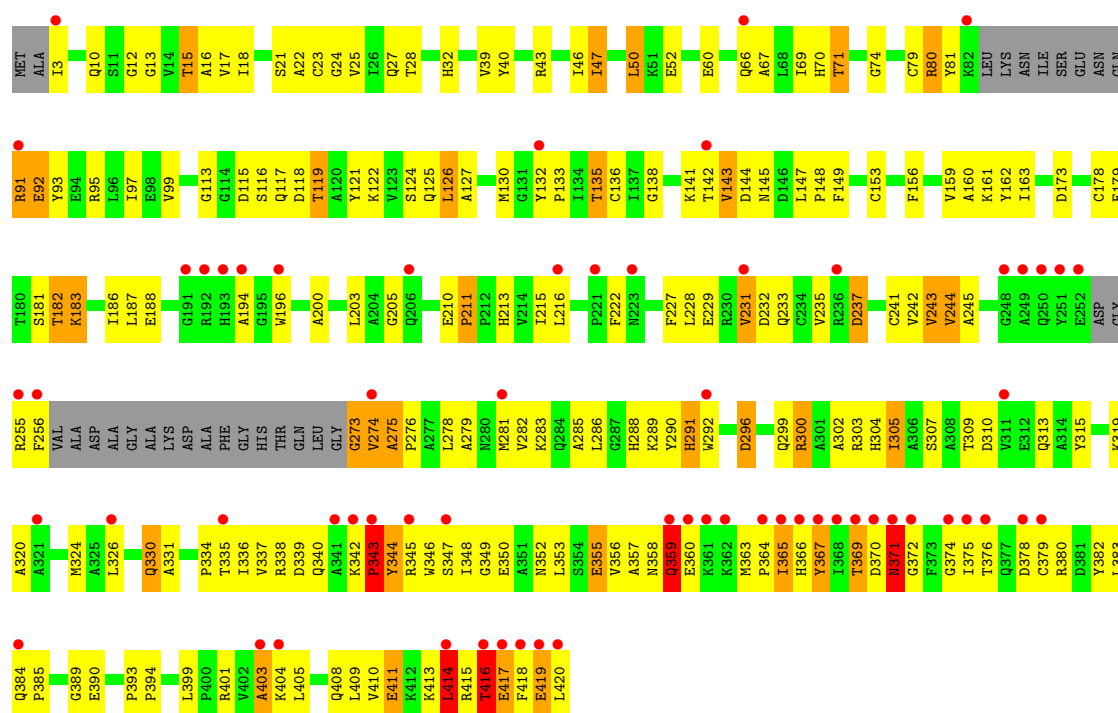
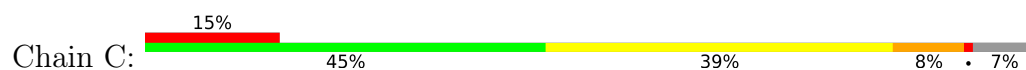


- Molecule 1: Pyrophosphate-dependent phosphofructokinase





● Molecule 1: Pyrophosphate-dependent phosphofructokinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.53Å 100.75Å 101.58Å 90.00° 110.34° 90.00°	Depositor
Resolution (Å)	44.70 – 2.50 44.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.9 (44.70-2.50) 90.6 (44.70-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.260 0.249 , 0.270	Depositor DCC
R_{free} test set	3762 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9397	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.18	39/3073 (1.3%)	1.03	16/4157 (0.4%)
1	B	1.00	19/3073 (0.6%)	0.95	9/4157 (0.2%)
1	C	0.58	6/3073 (0.2%)	0.96	13/4157 (0.3%)
All	All	0.95	64/9219 (0.7%)	0.98	38/12471 (0.3%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	LEU	C-O	-20.04	1.00	1.24
1	B	277	ALA	CA-CB	-19.86	1.22	1.53
1	B	275	ALA	C-O	-16.73	1.09	1.24
1	B	275	ALA	N-CA	-15.59	1.36	1.46
1	A	277	ALA	C-O	-15.45	1.06	1.24
1	B	420	LEU	C-OXT	14.50	1.52	1.23
1	A	274	VAL	C-O	-14.12	1.07	1.24
1	A	273	GLY	C-O	-13.12	0.97	1.23
1	A	360	GLU	C-O	-12.82	1.12	1.24
1	A	275	ALA	C-O	-12.81	1.11	1.24
1	B	275	ALA	CA-CB	-12.45	1.37	1.53
1	A	278	LEU	CA-C	-12.14	1.36	1.52
1	B	276	PRO	C-O	-12.00	1.08	1.24
1	A	361	LYS	CA-C	-11.51	1.40	1.53
1	B	274	VAL	C-O	-11.42	1.10	1.24
1	B	277	ALA	CA-C	-11.41	1.37	1.52
1	A	276	PRO	C-O	-11.25	1.10	1.24
1	A	277	ALA	CA-CB	-11.15	1.35	1.53
1	B	277	ALA	C-O	-10.90	1.10	1.24
1	A	361	LYS	C-O	-10.47	1.11	1.23
1	C	273	GLY	C-O	-10.07	1.03	1.23
1	A	275	ALA	CA-CB	-9.90	1.40	1.53
1	A	361	LYS	N-CA	-9.67	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	ALA	C-N	-8.96	1.21	1.33
1	B	276	PRO	CA-CB	-8.56	1.41	1.53
1	B	276	PRO	CG-CD	-8.51	1.21	1.50
1	C	275	ALA	CA-CB	-7.98	1.40	1.53
1	A	276	PRO	CB-CG	-7.91	1.10	1.49
1	A	273	GLY	C-N	-7.88	1.24	1.33
1	A	278	LEU	N-CA	-7.88	1.36	1.46
1	A	361	LYS	CD-CE	-7.87	1.28	1.52
1	B	276	PRO	CB-CG	-7.78	1.10	1.49
1	A	276	PRO	CG-CD	-7.74	1.24	1.50
1	C	275	ALA	C-O	-7.61	1.14	1.24
1	B	275	ALA	CA-C	-7.54	1.44	1.52
1	A	275	ALA	N-CA	-7.42	1.39	1.46
1	A	274	VAL	CA-C	-7.21	1.43	1.52
1	A	361	LYS	CE-NZ	-7.11	1.28	1.49
1	A	324	MET	SD-CE	-6.93	1.62	1.79
1	B	276	PRO	N-CA	-6.88	1.38	1.47
1	C	273	GLY	C-N	-6.62	1.26	1.33
1	A	273	GLY	CA-C	-6.44	1.40	1.52
1	A	275	ALA	C-N	-6.40	1.26	1.34
1	A	360	GLU	C-N	-6.39	1.24	1.33
1	A	276	PRO	C-N	-6.33	1.25	1.33
1	A	276	PRO	N-CA	-6.26	1.39	1.47
1	A	274	VAL	N-CA	-6.22	1.38	1.46
1	B	274	VAL	N-CA	-6.06	1.39	1.46
1	C	275	ALA	N-CA	-6.02	1.37	1.46
1	A	277	ALA	C-N	-5.97	1.26	1.33
1	A	277	ALA	CA-C	-5.96	1.45	1.52
1	A	278	LEU	CG-CD1	-5.87	1.33	1.52
1	C	275	ALA	CA-C	-5.84	1.45	1.52
1	B	276	PRO	C-N	-5.72	1.25	1.33
1	A	361	LYS	CB-CG	-5.70	1.35	1.52
1	A	274	VAL	C-N	-5.70	1.25	1.33
1	B	276	PRO	N-CD	-5.67	1.39	1.47
1	A	278	LEU	CA-CB	-5.54	1.44	1.53
1	A	361	LYS	CG-CD	-5.48	1.36	1.52
1	A	361	LYS	CA-CB	-5.46	1.45	1.52
1	A	277	ALA	N-CA	-5.39	1.40	1.46
1	A	359	GLN	N-CA	-5.37	1.39	1.45
1	A	276	PRO	N-CD	-5.37	1.40	1.47
1	B	276	PRO	CA-C	-5.37	1.44	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	GLU	CA-C-N	8.36	128.99	120.38
1	B	210	GLU	C-N-CA	8.36	128.99	120.38
1	A	210	GLU	CA-C-N	8.23	128.86	120.38
1	A	210	GLU	C-N-CA	8.23	128.86	120.38
1	C	274	VAL	N-CA-C	8.18	123.15	112.76
1	C	210	GLU	CA-C-N	7.96	128.58	120.38
1	C	210	GLU	C-N-CA	7.96	128.58	120.38
1	A	274	VAL	N-CA-C	7.46	118.26	110.72
1	B	322	VAL	N-CA-C	-7.38	103.27	110.72
1	B	371	ASN	N-CA-C	-7.05	103.61	111.71
1	A	276	PRO	CA-C-O	6.98	128.14	118.86
1	A	278	LEU	N-CA-C	6.86	119.63	111.33
1	C	92	GLU	N-CA-C	-6.81	103.78	111.14
1	C	371	ASN	N-CA-C	-6.75	104.00	111.36
1	B	92	GLU	N-CA-C	-6.68	103.93	111.14
1	A	92	GLU	N-CA-C	-6.51	104.11	111.14
1	A	360	GLU	CA-C-N	-6.02	113.44	122.47
1	A	360	GLU	C-N-CA	-6.02	113.44	122.47
1	C	211	PRO	N-CA-C	5.89	117.88	110.70
1	C	403	ALA	N-CA-C	5.77	117.43	111.03
1	A	211	PRO	N-CA-C	5.70	117.65	110.70
1	A	367	TYR	N-CA-C	-5.50	106.74	113.50
1	B	211	PRO	N-CA-C	5.49	117.39	110.70
1	C	372	GLY	N-CA-C	-5.46	107.57	115.27
1	B	20	ALA	N-CA-C	-5.42	105.45	111.36
1	A	410	VAL	N-CA-C	-5.36	102.00	109.45
1	C	47	ILE	N-CA-C	-5.33	104.55	110.62
1	C	378	ASP	N-CA-C	-5.26	105.46	111.14
1	C	367	TYR	N-CA-C	-5.25	107.42	113.88
1	B	276	PRO	CA-N-CD	-5.24	104.66	112.00
1	C	330	GLN	N-CA-C	5.22	117.32	109.23
1	C	296	ASP	CB-CA-C	-5.21	109.59	115.79
1	A	383	LEU	N-CA-C	5.17	117.92	111.24
1	A	393	PRO	CA-C-N	-5.12	114.68	119.85
1	A	393	PRO	C-N-CA	-5.12	114.68	119.85
1	A	276	PRO	CA-C-N	5.11	127.58	120.63
1	A	276	PRO	C-N-CA	5.11	127.58	120.63
1	B	47	ILE	N-CA-C	-5.01	104.79	111.05

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	3010	0	2950	181	0
1	B	3010	0	2950	202	0
1	C	3010	0	2950	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	136	0	0	15	0
3	B	109	0	0	13	0
3	C	119	0	0	15	0
All	All	9397	0	8850	587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (587) 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:C:15:THR:HG22	1:C:17:VAL:H	1.19	1.08
1:C:324:MET:HE3	1:C:350:GLU:HG2	1.35	1.07
1:B:15:THR:HG22	1:B:17:VAL:H	1.20	1.06
1:A:15:THR:HG22	1:A:17:VAL:H	1.19	1.03
1:B:342:LYS:HB2	1:B:343:PRO:HD2	1.38	1.02
1:C:28:THR:HG21	1:C:319:LYS:HG3	1.44	1.00
1:C:419:GLU:HG2	1:C:420:LEU:N	1.71	0.99
1:A:99:VAL:HG12	1:A:414:LEU:CD2	1.97	0.94
1:A:136:CYS:H	1:A:330:GLN:HE22	1.18	0.92
1:A:342:LYS:HB2	1:A:343:PRO:HD2	1.52	0.91
1:A:113:GLY:HA3	3:A:438:HOH:O	1.69	0.91
1:B:138:GLY:O	1:B:334:PRO:HD2	1.70	0.90
1:A:330:GLN:HE21	1:A:331:ALA:H	1.16	0.90
1:A:60:GLU:HG2	1:A:405:LEU:HD22	1.53	0.90
1:C:99:VAL:HG12	1:C:414:LEU:CD2	2.01	0.90
1:A:138:GLY:O	1:A:334:PRO:HD2	1.73	0.89
1:C:138:GLY:O	1:C:334:PRO:HD2	1.71	0.89
1:C:416:THR:HA	3:C:488:HOH:O	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ASN:N	1:A:371:ASN:HD22	1.72	0.86
1:A:375:ILE:HD11	1:A:379:CYS:SG	2.16	0.86
1:C:136:CYS:H	1:C:330:GLN:NE2	1.73	0.86
1:B:340:GLN:HG2	1:B:342:LYS:HG2	1.59	0.85
1:A:213:HIS:HD2	1:A:242:VAL:H	1.24	0.85
1:C:342:LYS:HB2	1:C:343:PRO:HD2	1.60	0.84
1:A:371:ASN:HD22	1:A:371:ASN:H	1.22	0.82
1:A:302:ALA:HB1	1:A:305:ILE:HD11	1.60	0.81
1:C:136:CYS:H	1:C:330:GLN:HE22	1.22	0.81
1:C:340:GLN:HG2	1:C:342:LYS:HG2	1.61	0.80
1:B:136:CYS:H	1:B:330:GLN:HE22	1.27	0.80
1:A:416:THR:HG22	1:A:417:GLU:H	1.47	0.80
1:C:302:ALA:HB1	1:C:305:ILE:HD11	1.64	0.80
1:B:213:HIS:HD2	1:B:242:VAL:H	1.27	0.80
1:C:213:HIS:HD2	1:C:242:VAL:H	1.27	0.80
1:B:416:THR:HG23	3:B:506:HOH:O	1.82	0.78
1:A:95:ARG:NH2	1:A:417:GLU:HB3	1.99	0.78
1:C:380:ARG:O	1:C:384:GLN:HG2	1.84	0.78
1:B:95:ARG:CZ	1:B:417:GLU:HB3	2.13	0.78
1:C:371:ASN:HD22	1:C:371:ASN:N	1.81	0.77
1:B:173:ASP:OD2	1:C:300:ARG:HD2	1.84	0.77
1:B:99:VAL:HG12	1:B:414:LEU:CD2	2.16	0.75
1:A:115:ASP:O	1:A:119:THR:HG22	1.87	0.75
1:B:115:ASP:O	1:B:119:THR:HG22	1.86	0.75
1:C:95:ARG:NH2	1:C:417:GLU:HB3	2.02	0.75
1:C:115:ASP:O	1:C:119:THR:HG22	1.87	0.74
1:C:302:ALA:HB1	1:C:305:ILE:CD1	2.17	0.74
1:A:13:GLY:H	1:A:80:ARG:HH21	1.33	0.74
1:B:13:GLY:H	1:B:80:ARG:HH21	1.34	0.74
1:B:371:ASN:ND2	1:B:371:ASN:H	1.84	0.73
1:C:15:THR:HG22	1:C:17:VAL:N	2.00	0.73
1:B:95:ARG:NE	1:B:417:GLU:HG2	2.03	0.73
1:A:15:THR:HG22	1:A:17:VAL:N	2.01	0.73
1:B:70:HIS:HB2	1:B:393:PRO:HB3	1.69	0.73
1:C:125:GLN:HG3	3:C:525:HOH:O	1.89	0.73
1:C:143:VAL:HG22	1:C:159:VAL:HG11	1.71	0.72
1:B:309:THR:O	1:B:313:GLN:HG3	1.89	0.72
1:A:118:ASP:OD1	1:A:122:LYS:HE2	1.90	0.72
1:B:202:GLY:HA3	1:B:375:ILE:HD12	1.72	0.72
1:B:213:HIS:CD2	1:B:241:CYS:HA	2.24	0.72
1:B:302:ALA:HB1	1:B:305:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASP:O	1:B:299:GLN:HG2	1.90	0.71
1:B:371:ASN:N	1:B:371:ASN:HD22	1.89	0.71
1:C:118:ASP:OD1	1:C:122:LYS:HE2	1.90	0.71
1:C:358:ASN:O	1:C:359:GLN:CG	2.38	0.71
1:C:235:VAL:HG21	1:C:288:HIS:NE2	2.06	0.71
1:C:213:HIS:CD2	1:C:241:CYS:HA	2.26	0.70
1:C:99:VAL:HG12	1:C:414:LEU:HD22	1.73	0.70
1:C:95:ARG:NE	1:C:417:GLU:HG2	2.06	0.69
1:C:142:THR:HG22	1:C:144:ASP:H	1.56	0.69
1:C:24:GLY:O	1:C:28:THR:HG23	1.92	0.69
1:B:371:ASN:ND2	1:B:371:ASN:N	2.38	0.69
1:A:24:GLY:O	1:A:28:THR:HG23	1.92	0.69
1:A:235:VAL:HG21	1:A:288:HIS:NE2	2.08	0.69
1:C:28:THR:HG21	1:C:319:LYS:CG	2.21	0.69
1:B:15:THR:HG22	1:B:17:VAL:N	2.02	0.69
1:C:419:GLU:HG2	1:C:420:LEU:H	1.56	0.69
1:C:324:MET:CE	1:C:350:GLU:HG2	2.20	0.69
1:A:296:ASP:O	1:A:299:GLN:HG2	1.93	0.69
1:C:60:GLU:HG2	1:C:405:LEU:HD22	1.74	0.69
1:A:13:GLY:H	1:A:80:ARG:NH2	1.91	0.69
1:B:136:CYS:H	1:B:330:GLN:NE2	1.91	0.69
1:C:13:GLY:H	1:C:80:ARG:HH21	1.39	0.69
1:B:235:VAL:HG21	1:B:288:HIS:NE2	2.07	0.68
1:B:358:ASN:O	1:B:359:GLN:HG2	1.93	0.68
1:A:142:THR:HG22	1:A:144:ASP:H	1.56	0.68
1:B:118:ASP:OD1	1:B:122:LYS:HE2	1.93	0.68
1:C:27:GLN:HE22	1:C:66:GLN:NE2	1.91	0.68
1:B:27:GLN:HE22	1:B:66:GLN:NE2	1.91	0.68
1:A:67:ALA:O	1:A:71:THR:HG22	1.94	0.68
1:A:213:HIS:CD2	1:A:241:CYS:HA	2.28	0.68
1:B:60:GLU:HG2	1:B:405:LEU:HD22	1.75	0.68
1:A:309:THR:O	1:A:313:GLN:HG3	1.93	0.67
1:B:143:VAL:HG22	1:B:159:VAL:HG11	1.77	0.67
1:B:13:GLY:H	1:B:80:ARG:NH2	1.92	0.67
1:B:305:ILE:HD12	1:B:305:ILE:H	1.58	0.67
1:B:142:THR:HG22	1:B:144:ASP:H	1.58	0.67
1:A:27:GLN:HE22	1:A:66:GLN:NE2	1.92	0.67
1:A:309:THR:HG23	1:A:388:ALA:O	1.94	0.67
1:B:135:THR:HA	1:B:330:GLN:OE1	1.95	0.67
1:A:330:GLN:HE21	1:A:331:ALA:N	1.91	0.67
1:C:274:VAL:HG12	1:C:274:VAL:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:PRO:HG3	1:C:359:GLN:O	1.95	0.67
1:A:95:ARG:CZ	1:A:417:GLU:HB3	2.25	0.66
1:A:342:LYS:O	1:A:343:PRO:C	2.38	0.66
1:C:194:ALA:HB1	3:C:432:HOH:O	1.95	0.66
1:B:203:LEU:HD12	1:B:384:GLN:OE1	1.96	0.66
1:A:302:ALA:HB1	1:A:305:ILE:CD1	2.24	0.66
1:A:118:ASP:HB2	1:A:357:ALA:HB2	1.77	0.66
1:A:136:CYS:H	1:A:330:GLN:NE2	1.93	0.66
1:B:67:ALA:O	1:B:71:THR:HG22	1.95	0.65
1:C:118:ASP:HB2	1:C:357:ALA:HB2	1.79	0.65
1:C:371:ASN:N	1:C:371:ASN:ND2	2.44	0.65
1:A:283:LYS:HD2	1:A:290:TYR:HE1	1.62	0.65
1:B:24:GLY:O	1:B:28:THR:HG23	1.97	0.65
1:C:13:GLY:H	1:C:80:ARG:NH2	1.95	0.65
1:C:367:TYR:O	1:C:376:THR:HG23	1.96	0.65
1:A:99:VAL:HG12	1:A:414:LEU:HD22	1.77	0.64
1:B:95:ARG:NH2	1:B:417:GLU:HB3	2.12	0.64
1:C:67:ALA:O	1:C:71:THR:HG22	1.97	0.64
1:B:302:ALA:HB1	1:B:305:ILE:HD11	1.78	0.64
1:C:342:LYS:O	1:C:343:PRO:C	2.39	0.64
1:B:307:SER:HB3	1:B:310:ASP:HB2	1.80	0.64
1:C:70:HIS:HB2	1:C:393:PRO:HB3	1.80	0.64
1:C:418:PHE:HA	3:C:511:HOH:O	1.97	0.64
1:C:283:LYS:HD2	1:C:290:TYR:HE1	1.63	0.64
1:C:232:ASP:HB2	1:C:286:LEU:HD13	1.80	0.64
1:A:95:ARG:NH1	1:A:414:LEU:HD23	2.13	0.63
1:B:417:GLU:HG3	1:B:417:GLU:O	1.97	0.63
1:C:342:LYS:CB	1:C:343:PRO:HD2	2.28	0.63
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.64	0.63
1:A:136:CYS:N	1:A:330:GLN:HE22	1.94	0.63
1:B:415:ARG:HB2	3:B:468:HOH:O	1.99	0.62
1:B:342:LYS:CB	1:B:343:PRO:HD2	2.22	0.62
1:A:371:ASN:H	1:A:371:ASN:ND2	1.91	0.62
1:C:324:MET:HE3	1:C:350:GLU:CG	2.22	0.62
1:A:10:GLN:HE22	1:A:74:GLY:CA	2.12	0.62
1:B:199:ALA:O	1:B:375:ILE:HD11	1.99	0.62
1:B:283:LYS:HD2	1:B:290:TYR:HE1	1.63	0.62
1:B:10:GLN:HE22	1:B:74:GLY:CA	2.12	0.62
1:B:27:GLN:HE22	1:B:66:GLN:HE21	1.48	0.62
1:A:416:THR:HG22	1:A:417:GLU:N	2.13	0.62
1:C:10:GLN:HE22	1:C:74:GLY:CA	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:CYS:N	1:C:330:GLN:HE22	1.94	0.61
1:B:232:ASP:HB2	1:B:286:LEU:HD13	1.82	0.61
1:C:211:PRO:HB3	1:C:242:VAL:HG21	1.82	0.61
1:A:91:ARG:N	3:A:423:HOH:O	2.33	0.61
1:B:342:LYS:O	1:B:344:TYR:N	2.33	0.61
1:A:50:LEU:O	1:A:417:GLU:HG2	2.00	0.61
1:A:91:ARG:HG3	1:A:92:GLU:H	1.65	0.61
1:B:99:VAL:HG12	1:B:414:LEU:HD22	1.83	0.61
1:C:417:GLU:O	1:C:417:GLU:HG3	2.00	0.61
1:C:331:ALA:HA	1:C:353:LEU:HD12	1.83	0.61
1:B:141:LYS:C	1:B:141:LYS:HD2	2.27	0.60
1:B:342:LYS:O	1:B:343:PRO:C	2.44	0.60
1:A:322:VAL:O	1:A:326:LEU:HD22	2.01	0.60
1:B:91:ARG:HG3	1:B:92:GLU:H	1.66	0.60
1:B:396:ASP:O	1:B:397:ASP:HB2	2.01	0.60
1:C:91:ARG:HG3	1:C:92:GLU:H	1.66	0.60
1:C:358:ASN:O	1:C:359:GLN:HG3	2.02	0.60
1:A:47:ILE:HD11	1:A:81:TYR:CG	2.37	0.60
1:A:27:GLN:HE22	1:A:66:GLN:HE21	1.50	0.60
1:A:138:GLY:O	1:A:334:PRO:CD	2.48	0.59
1:A:232:ASP:HB2	1:A:286:LEU:HD13	1.84	0.59
1:A:357:ALA:HB3	3:A:510:HOH:O	2.01	0.59
1:C:161:LYS:NZ	1:C:390:GLU:HG3	2.17	0.59
1:C:27:GLN:HE22	1:C:66:GLN:HE21	1.48	0.59
1:C:47:ILE:HD11	1:C:81:TYR:CG	2.38	0.59
1:A:403:ALA:O	1:A:404:LYS:HB2	2.02	0.58
1:C:182:THR:HG21	1:C:291:HIS:CD2	2.38	0.58
1:C:382:TYR:O	1:C:385:PRO:HD2	2.03	0.58
1:A:375:ILE:CD1	1:A:379:CYS:SG	2.91	0.58
1:B:47:ILE:HD11	1:B:81:TYR:CG	2.39	0.58
1:C:279:ALA:HB1	1:C:290:TYR:CD2	2.39	0.58
1:A:15:THR:CG2	1:A:16:ALA:N	2.67	0.58
1:B:279:ALA:HB1	1:B:290:TYR:CD2	2.38	0.58
1:B:342:LYS:HB2	1:B:343:PRO:CD	2.23	0.58
1:C:216:LEU:HD12	1:C:278:LEU:HD11	1.84	0.58
1:B:300:ARG:HD3	1:C:173:ASP:OD2	2.04	0.57
1:A:141:LYS:HD2	1:A:141:LYS:C	2.30	0.57
1:C:364:PRO:HB2	1:C:366:HIS:CD2	2.39	0.57
1:C:296:ASP:O	1:C:299:GLN:HG2	2.04	0.57
1:B:116:SER:O	1:B:119:THR:HG23	2.04	0.57
1:A:18:ILE:HD12	1:A:141:LYS:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:CG	1:A:405:LEU:HD22	2.32	0.57
1:A:329:LYS:NZ	1:B:340:GLN:HG3	2.20	0.57
1:A:295:ALA:O	1:A:298:LEU:HB2	2.04	0.57
1:A:21:SER:O	1:A:25:VAL:HG12	2.04	0.57
1:C:50:LEU:O	1:C:417:GLU:HG2	2.05	0.57
1:A:335:THR:O	1:A:348:ILE:HA	2.05	0.56
1:C:156:PHE:CE2	1:C:196:TRP:HB3	2.40	0.56
1:C:145:ASN:HA	1:C:153:CYS:SG	2.45	0.56
1:A:375:ILE:HG13	1:A:379:CYS:HB3	1.86	0.56
1:C:15:THR:CG2	1:C:16:ALA:N	2.69	0.56
1:C:141:LYS:HD2	1:C:141:LYS:C	2.31	0.56
1:A:24:GLY:HA2	1:A:315:TYR:CE1	2.41	0.56
1:A:70:HIS:HB2	1:A:393:PRO:HB3	1.88	0.56
1:B:18:ILE:HD12	1:B:141:LYS:HG3	1.88	0.56
1:B:200:ALA:HA	1:B:203:LEU:HD23	1.88	0.56
1:C:313:GLN:HE21	1:C:346:TRP:CG	2.23	0.55
1:B:211:PRO:HB3	1:B:242:VAL:HG21	1.88	0.55
1:A:147:LEU:HB2	1:A:153:CYS:SG	2.45	0.55
1:A:305:ILE:HD12	1:A:305:ILE:H	1.71	0.55
1:B:337:VAL:HG22	1:B:347:SER:O	2.07	0.55
1:C:18:ILE:HD12	1:C:141:LYS:HG3	1.87	0.55
1:C:3:ILE:HG23	1:C:3:ILE:O	2.06	0.55
1:B:380:ARG:HG3	1:B:380:ARG:NH1	2.20	0.55
1:C:200:ALA:HA	1:C:203:LEU:HD23	1.88	0.55
1:B:216:LEU:HD12	1:B:278:LEU:HD11	1.89	0.55
1:A:186:ILE:HG12	1:A:243:VAL:HG22	1.89	0.55
1:A:200:ALA:HA	1:A:203:LEU:HD23	1.89	0.55
1:C:320:ALA:HB1	1:C:348:ILE:HG21	1.89	0.55
1:A:59:LEU:HB3	3:A:483:HOH:O	2.08	0.54
1:A:279:ALA:HB1	1:A:290:TYR:CD2	2.42	0.54
1:B:10:GLN:NE2	3:B:430:HOH:O	2.40	0.54
1:A:182:THR:HG21	1:A:291:HIS:CD2	2.42	0.54
1:B:186:ILE:HG12	1:B:243:VAL:HG22	1.90	0.54
1:B:320:ALA:HB1	1:B:348:ILE:HG21	1.90	0.54
1:B:199:ALA:O	1:B:375:ILE:CD1	2.55	0.54
1:B:338:ARG:NH1	1:B:344:TYR:CE1	2.75	0.54
1:B:147:LEU:HB2	1:B:153:CYS:SG	2.48	0.54
1:B:340:GLN:HG2	1:B:342:LYS:CG	2.36	0.54
1:C:355:GLU:HB3	3:C:515:HOH:O	2.08	0.54
1:A:10:GLN:NE2	3:A:422:HOH:O	2.40	0.54
1:C:142:THR:HA	3:C:502:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASN:O	1:B:359:GLN:CG	2.56	0.54
1:C:116:SER:O	1:C:119:THR:HG23	2.07	0.54
1:C:127:ALA:HB1	1:C:132:TYR:O	2.05	0.54
1:C:135:THR:HA	1:C:330:GLN:HE22	1.74	0.53
1:C:419:GLU:CG	1:C:420:LEU:N	2.53	0.53
1:A:116:SER:O	1:A:119:THR:HG23	2.09	0.53
1:A:365:ILE:C	1:A:367:TYR:H	2.16	0.53
1:A:275:ALA:HB3	1:A:276:PRO:CD	2.39	0.53
1:C:196:TRP:CD1	3:C:432:HOH:O	2.61	0.53
1:B:300:ARG:CD	1:C:173:ASP:OD2	2.57	0.53
1:A:291:HIS:HB2	3:A:424:HOH:O	2.08	0.53
1:A:371:ASN:N	1:A:371:ASN:ND2	2.45	0.53
1:B:127:ALA:HB1	1:B:132:TYR:O	2.09	0.53
1:C:95:ARG:CZ	1:C:417:GLU:CB	2.86	0.53
1:C:338:ARG:NH1	1:C:344:TYR:CD1	2.77	0.53
1:A:211:PRO:HB3	1:A:242:VAL:HG21	1.89	0.53
1:B:307:SER:HB3	1:B:310:ASP:CB	2.39	0.53
1:C:143:VAL:HG22	1:C:159:VAL:CG1	2.37	0.53
1:C:178:CYS:O	1:C:183:LYS:HE2	2.08	0.53
1:A:93:TYR:HB3	1:A:126:LEU:HD12	1.91	0.53
1:B:305:ILE:HD12	1:B:305:ILE:N	2.21	0.52
1:C:135:THR:HA	1:C:330:GLN:NE2	2.24	0.52
1:A:143:VAL:HG22	1:A:159:VAL:HG11	1.91	0.52
1:A:348:ILE:N	1:A:348:ILE:HD12	2.23	0.52
1:B:15:THR:CG2	1:B:16:ALA:N	2.72	0.52
1:B:227:PHE:O	1:B:231:VAL:HG12	2.10	0.52
1:C:95:ARG:HE	1:C:417:GLU:HG2	1.75	0.52
1:A:127:ALA:HB1	1:A:132:TYR:O	2.09	0.52
1:B:186:ILE:O	1:B:292:TRP:HA	2.09	0.52
1:C:274:VAL:O	1:C:274:VAL:CG1	2.56	0.52
1:C:309:THR:O	1:C:313:GLN:HG3	2.09	0.52
1:A:330:GLN:NE2	1:A:331:ALA:H	1.97	0.52
1:A:227:PHE:O	1:A:231:VAL:HG12	2.10	0.52
1:B:177:MET:HE1	1:C:300:ARG:HH12	1.76	0.51
1:B:320:ALA:CB	1:B:348:ILE:HG21	2.40	0.51
1:C:21:SER:O	1:C:25:VAL:HG12	2.10	0.51
1:C:93:TYR:HB3	1:C:126:LEU:HD12	1.92	0.51
1:A:99:VAL:HG12	1:A:414:LEU:HD21	1.85	0.51
1:A:178:CYS:O	1:A:183:LYS:HE2	2.10	0.51
1:A:290:TYR:C	3:A:424:HOH:O	2.54	0.51
1:B:70:HIS:HB2	1:B:393:PRO:CB	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:VAL:HG13	1:C:232:ASP:H	1.76	0.51
1:A:40:TYR:CE1	1:A:410:VAL:HG21	2.46	0.51
1:B:23:CYS:SG	1:B:69:ILE:CG2	2.99	0.51
1:A:4:LYS:NZ	3:A:455:HOH:O	2.44	0.51
1:B:355:GLU:C	1:B:357:ALA:N	2.68	0.51
1:C:182:THR:HG21	1:C:291:HIS:HD2	1.76	0.51
1:A:199:ALA:HB1	1:A:375:ILE:HD11	1.93	0.51
1:B:196:TRP:CE3	1:B:363:MET:HE3	2.46	0.51
1:C:320:ALA:CB	1:C:348:ILE:HG21	2.41	0.51
1:C:330:GLN:HE21	1:C:331:ALA:H	1.59	0.51
1:A:10:GLN:HE22	1:A:74:GLY:HA2	1.75	0.51
1:A:95:ARG:CZ	1:A:417:GLU:CB	2.88	0.51
1:A:316:ALA:HB1	1:A:348:ILE:HD11	1.93	0.51
1:B:95:ARG:HE	1:B:417:GLU:HG2	1.74	0.51
3:B:507:HOH:O	1:C:305:ILE:HG23	2.11	0.51
1:C:161:LYS:HE3	1:C:389:GLY:O	2.11	0.51
1:C:313:GLN:HB3	1:C:336:ILE:HD12	1.92	0.51
1:A:291:HIS:N	3:A:424:HOH:O	2.44	0.50
1:A:340:GLN:O	1:A:344:TYR:HA	2.10	0.50
1:B:178:CYS:O	1:B:183:LYS:HE2	2.11	0.50
1:B:185:PHE:HA	1:B:291:HIS:O	2.10	0.50
1:C:337:VAL:O	1:C:346:TRP:HA	2.11	0.50
1:B:71:THR:HG21	1:B:403:ALA:HB2	1.92	0.50
1:B:117:GLN:HE21	1:B:333:MET:HB2	1.77	0.50
1:B:30:ARG:HB3	3:B:449:HOH:O	2.10	0.50
1:C:52:GLU:OE1	1:C:413:LYS:N	2.40	0.50
1:A:383:LEU:C	1:A:385:PRO:HD2	2.37	0.50
1:C:349:GLY:O	1:C:350:GLU:HG3	2.12	0.50
1:A:327:ALA:HB1	1:B:339:ASP:O	2.11	0.50
1:B:21:SER:O	1:B:25:VAL:HG12	2.11	0.50
1:C:186:ILE:HG12	1:C:243:VAL:HG22	1.92	0.50
1:C:255:ARG:HB3	1:C:256:PHE:HD1	1.75	0.50
1:B:279:ALA:O	1:B:282:VAL:HG22	2.11	0.50
1:C:91:ARG:CG	1:C:92:GLU:H	2.25	0.50
1:C:419:GLU:CG	1:C:420:LEU:H	2.20	0.50
1:B:93:TYR:HB3	1:B:126:LEU:HD12	1.93	0.50
1:C:273:GLY:O	1:C:276:PRO:HD2	2.11	0.50
1:A:182:THR:HG21	1:A:291:HIS:HD2	1.75	0.50
1:B:143:VAL:HG22	1:B:159:VAL:CG1	2.41	0.50
1:B:200:ALA:O	1:B:203:LEU:HD23	2.12	0.50
1:B:231:VAL:HG13	1:B:232:ASP:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:CZ	1:C:417:GLU:HB3	2.42	0.50
1:C:292:TRP:CD1	1:C:292:TRP:C	2.89	0.50
1:C:367:TYR:C	1:C:376:THR:HG23	2.37	0.50
1:A:91:ARG:CG	1:A:92:GLU:H	2.24	0.49
1:A:255:ARG:HB3	1:A:256:PHE:HD1	1.77	0.49
1:A:417:GLU:O	1:A:417:GLU:HG3	2.10	0.49
1:C:121:TYR:O	1:C:124:SER:HB3	2.12	0.49
1:C:147:LEU:HB2	1:C:153:CYS:SG	2.53	0.49
1:B:125:GLN:NE2	3:B:529:HOH:O	2.44	0.49
1:B:213:HIS:CD2	1:B:242:VAL:H	2.18	0.49
1:B:10:GLN:HE22	1:B:74:GLY:HA2	1.77	0.49
1:B:10:GLN:HE22	1:B:74:GLY:HA3	1.77	0.49
1:B:91:ARG:CG	1:B:92:GLU:H	2.25	0.49
1:C:342:LYS:O	1:C:344:TYR:N	2.45	0.49
1:C:360:GLU:HB3	3:C:506:HOH:O	2.11	0.49
1:A:23:CYS:SG	1:A:69:ILE:CG2	3.00	0.49
1:B:316:ALA:HB1	1:B:348:ILE:HD11	1.94	0.49
1:C:10:GLN:HE22	1:C:74:GLY:HA2	1.77	0.49
1:B:216:LEU:HA	3:B:517:HOH:O	2.12	0.49
1:B:357:ALA:O	1:B:358:ASN:HB2	2.12	0.49
1:C:233:GLN:O	1:C:237:ASP:HB2	2.12	0.49
1:B:317:VAL:O	1:B:334:PRO:HG3	2.13	0.49
1:C:23:CYS:SG	1:C:69:ILE:CG2	3.01	0.49
1:C:162:TYR:HD2	1:C:163:ILE:HD12	1.77	0.49
1:C:279:ALA:O	1:C:282:VAL:HG22	2.11	0.49
1:A:15:THR:HG22	1:A:16:ALA:N	2.28	0.49
1:C:330:GLN:HG3	1:C:331:ALA:N	2.26	0.49
1:A:231:VAL:HG13	1:A:232:ASP:H	1.78	0.49
1:C:126:LEU:HD22	1:C:130:MET:HG3	1.94	0.49
1:C:384:GLN:HG3	1:C:385:PRO:HD3	1.94	0.49
1:A:158:SER:HB3	3:A:453:HOH:O	2.13	0.48
1:A:380:ARG:HD3	3:A:470:HOH:O	2.11	0.48
1:C:159:VAL:CG2	1:C:160:ALA:N	2.76	0.48
1:A:162:TYR:HD2	1:A:163:ILE:HD12	1.77	0.48
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.94	0.48
1:A:411:GLU:O	1:A:412:LYS:O	2.30	0.48
1:C:10:GLN:HE22	1:C:74:GLY:HA3	1.79	0.48
1:C:40:TYR:CE1	1:C:410:VAL:HG21	2.48	0.48
1:C:307:SER:HB3	1:C:310:ASP:HB2	1.95	0.48
1:C:363:MET:HB2	3:C:432:HOH:O	2.12	0.48
1:C:394:PRO:HG3	1:C:401:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HG2	3:A:423:HOH:O	2.12	0.48
1:B:119:THR:HG21	3:B:422:HOH:O	2.12	0.48
1:B:255:ARG:HB3	1:B:256:PHE:HD1	1.78	0.48
1:C:28:THR:CG2	1:C:319:LYS:HG3	2.27	0.48
1:B:162:TYR:HD2	1:B:163:ILE:HD12	1.78	0.48
1:C:149:PHE:O	1:C:335:THR:HG21	2.14	0.48
1:B:296:ASP:CG	1:B:297:TYR:H	2.21	0.48
1:B:375:ILE:HG23	1:B:379:CYS:HB3	1.96	0.48
1:C:70:HIS:HA	1:C:303:ARG:CZ	2.43	0.48
1:C:126:LEU:CD2	1:C:130:MET:HG3	2.44	0.48
1:C:371:ASN:ND2	1:C:371:ASN:H	2.09	0.48
1:A:340:GLN:HG2	1:A:342:LYS:HG3	1.95	0.48
1:C:81:TYR:CZ	1:C:419:GLU:HG3	2.48	0.48
1:A:369:THR:HG23	1:A:374:GLY:C	2.38	0.48
1:B:4:LYS:NZ	1:B:4:LYS:HB2	2.29	0.48
1:C:133:PRO:HA	3:C:441:HOH:O	2.12	0.48
1:A:126:LEU:CD2	1:A:130:MET:HG3	2.43	0.48
1:A:215:ILE:HG12	1:A:244:VAL:CG1	2.44	0.48
1:A:279:ALA:O	1:A:282:VAL:HG22	2.13	0.48
1:B:308:ALA:HB2	1:B:390:GLU:O	2.14	0.48
1:A:71:THR:HG21	1:A:403:ALA:HB2	1.96	0.48
1:A:233:GLN:O	1:A:237:ASP:HB2	2.14	0.48
1:A:360:GLU:OE1	1:A:362:LYS:HD2	2.14	0.47
1:B:121:TYR:O	1:B:124:SER:HB3	2.13	0.47
1:B:233:GLN:O	1:B:237:ASP:HB2	2.14	0.47
1:C:39:VAL:HG23	3:C:462:HOH:O	2.13	0.47
1:A:161:LYS:NZ	1:A:390:GLU:HG3	2.30	0.47
1:A:296:ASP:CG	1:A:297:TYR:H	2.22	0.47
1:A:135:THR:HA	1:A:330:GLN:HE22	1.79	0.47
1:A:342:LYS:O	1:A:344:TYR:N	2.47	0.47
1:B:242:VAL:O	1:B:242:VAL:HG23	2.13	0.47
1:C:24:GLY:HA2	1:C:315:TYR:CE1	2.49	0.47
1:C:215:ILE:HG12	1:C:244:VAL:CG1	2.44	0.47
1:C:242:VAL:HG23	1:C:242:VAL:O	2.13	0.47
1:B:415:ARG:O	1:B:416:THR:O	2.32	0.47
1:C:339:ASP:N	1:C:345:ARG:O	2.48	0.47
1:A:21:SER:HA	1:A:314:ALA:O	2.15	0.47
1:A:47:ILE:HG12	1:A:79:CYS:SG	2.55	0.47
1:B:12:GLY:HA2	1:B:80:ARG:HE	1.79	0.47
1:B:297:TYR:OH	1:C:182:THR:HG21	2.15	0.47
1:B:322:VAL:O	1:B:325:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PHE:O	1:C:231:VAL:HG12	2.14	0.47
1:A:126:LEU:HD22	1:A:130:MET:HG3	1.97	0.47
1:A:341:ALA:C	1:A:342:LYS:O	2.54	0.47
1:B:28:THR:HG21	1:B:319:LYS:HG3	1.97	0.47
1:C:15:THR:CG2	1:C:17:VAL:H	2.08	0.47
1:A:213:HIS:CD2	1:A:242:VAL:H	2.16	0.46
1:A:347:SER:HB2	3:A:448:HOH:O	2.16	0.46
1:A:133:PRO:HA	3:A:467:HOH:O	2.15	0.46
1:A:199:ALA:HB1	1:A:375:ILE:CD1	2.46	0.46
1:A:364:PRO:O	1:A:367:TYR:HB2	2.15	0.46
1:C:200:ALA:O	1:C:203:LEU:HD23	2.15	0.46
1:B:297:TYR:CE1	1:B:300:ARG:NH1	2.84	0.46
1:C:97:ILE:HD13	1:C:127:ALA:HA	1.97	0.46
1:B:126:LEU:HD22	1:B:130:MET:HG3	1.98	0.46
1:C:285:ALA:O	1:C:286:LEU:HD23	2.16	0.46
1:B:126:LEU:CD2	1:B:130:MET:HG3	2.45	0.46
1:B:215:ILE:HG12	1:B:244:VAL:CG1	2.45	0.46
1:C:32:HIS:CG	1:C:326:LEU:HD21	2.51	0.46
1:C:182:THR:N	1:C:289:LYS:HD3	2.30	0.46
1:B:60:GLU:CG	1:B:405:LEU:HD22	2.44	0.46
1:B:95:ARG:CZ	1:B:417:GLU:CB	2.91	0.46
1:C:161:LYS:HZ2	1:C:390:GLU:HG3	1.81	0.46
1:A:302:ALA:O	1:A:305:ILE:HD12	2.16	0.46
1:A:357:ALA:O	1:A:358:ASN:HB2	2.15	0.46
1:B:297:TYR:O	1:B:300:ARG:HG3	2.15	0.46
1:C:91:ARG:HE	1:C:91:ARG:HB3	1.10	0.46
1:A:121:TYR:O	1:A:124:SER:HB3	2.16	0.46
1:A:242:VAL:O	1:A:242:VAL:HG23	2.15	0.46
1:B:222:PHE:CE2	1:B:281:MET:HE1	2.51	0.46
1:B:228:LEU:HD11	1:B:281:MET:HB3	1.97	0.46
1:C:12:GLY:HA2	1:C:80:ARG:HE	1.80	0.46
1:C:337:VAL:CG2	1:C:347:SER:OG	2.64	0.46
1:A:12:GLY:HA2	1:A:80:ARG:HE	1.81	0.46
1:A:375:ILE:CG1	1:A:379:CYS:SG	3.04	0.46
1:A:307:SER:O	1:A:311:VAL:HG13	2.16	0.45
1:C:365:ILE:C	1:C:367:TYR:H	2.23	0.45
1:A:329:LYS:HZ3	1:B:340:GLN:HG3	1.79	0.45
1:C:302:ALA:O	1:C:305:ILE:HD12	2.16	0.45
1:A:228:LEU:HD11	1:A:281:MET:HB3	1.99	0.45
1:B:367:TYR:O	1:B:376:THR:HG23	2.16	0.45
1:C:213:HIS:CD2	1:C:242:VAL:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:HIS:CD2	1:B:401:ARG:O	2.70	0.45
1:C:231:VAL:HG13	1:C:232:ASP:N	2.32	0.45
1:A:161:LYS:HE3	1:A:389:GLY:O	2.16	0.45
1:C:15:THR:HG22	1:C:16:ALA:N	2.31	0.45
1:A:22:ALA:HA	1:A:25:VAL:CG1	2.47	0.45
1:C:380:ARG:HG3	1:C:380:ARG:HH11	1.82	0.45
1:B:99:VAL:HG12	1:B:414:LEU:HD23	1.95	0.45
1:B:223:ASN:CB	3:B:490:HOH:O	2.64	0.45
1:B:331:ALA:C	1:B:353:LEU:HG	2.42	0.45
1:B:338:ARG:NH1	1:B:344:TYR:CD1	2.83	0.44
1:C:313:GLN:HB3	1:C:336:ILE:CD1	2.48	0.44
1:A:60:GLU:CD	1:A:406:LYS:H	2.26	0.44
1:B:28:THR:O	1:B:32:HIS:HD2	2.00	0.44
1:B:143:VAL:CG2	1:B:159:VAL:HG11	2.45	0.44
1:B:314:ALA:O	1:B:317:VAL:HG22	2.17	0.44
1:B:292:TRP:CD1	1:B:292:TRP:C	2.95	0.44
1:C:47:ILE:HG12	1:C:79:CYS:SG	2.57	0.44
1:C:148:PRO:CG	1:C:359:GLN:O	2.65	0.44
1:C:255:ARG:HB3	1:C:256:PHE:CD1	2.52	0.44
1:C:375:ILE:HD11	1:C:379:CYS:SG	2.58	0.44
1:B:222:PHE:HE2	1:B:281:MET:HE1	1.82	0.44
1:B:355:GLU:C	1:B:357:ALA:H	2.25	0.44
1:A:52:GLU:OE2	1:A:414:LEU:HB2	2.18	0.44
1:B:50:LEU:O	1:B:417:GLU:HG2	2.17	0.44
1:B:81:TYR:OH	1:B:419:GLU:HB2	2.18	0.44
1:B:213:HIS:HD2	1:B:242:VAL:N	2.05	0.44
1:C:118:ASP:HB2	1:C:357:ALA:CB	2.46	0.44
1:C:196:TRP:CE3	1:C:363:MET:HE3	2.52	0.44
1:C:352:ASN:O	1:C:356:VAL:HG23	2.18	0.44
1:B:331:ALA:O	1:B:353:LEU:HG	2.18	0.44
1:C:28:THR:O	1:C:32:HIS:HD2	2.01	0.44
1:B:47:ILE:HG12	1:B:79:CYS:SG	2.57	0.44
1:B:231:VAL:HG13	1:B:232:ASP:N	2.33	0.44
1:B:326:LEU:N	1:B:326:LEU:CD1	2.80	0.44
1:C:70:HIS:HA	1:C:303:ARG:NH2	2.33	0.44
1:C:143:VAL:CG2	1:C:159:VAL:HG11	2.46	0.44
1:C:91:ARG:N	3:C:436:HOH:O	2.51	0.44
1:C:364:PRO:O	1:C:367:TYR:HB2	2.18	0.44
1:A:97:ILE:HD13	1:A:127:ALA:HA	2.00	0.43
1:B:97:ILE:HD13	1:B:127:ALA:HA	1.99	0.43
1:B:308:ALA:C	1:B:310:ASP:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:HG23	1:C:243:VAL:CG2	2.48	0.43
1:B:161:LYS:HE3	1:B:389:GLY:O	2.18	0.43
1:A:182:THR:HA	1:A:289:LYS:HB3	2.00	0.43
1:A:210:GLU:HA	1:A:211:PRO:HD3	1.81	0.43
1:B:52:GLU:OE2	1:B:414:LEU:HB2	2.19	0.43
1:C:222:PHE:CE2	1:C:281:MET:HE1	2.53	0.43
1:C:403:ALA:O	1:C:404:LYS:HB2	2.18	0.43
1:A:188:GLU:HA	1:A:245:ALA:O	2.18	0.43
1:B:182:THR:HA	1:B:289:LYS:HB3	2.00	0.43
1:C:188:GLU:HA	1:C:245:ALA:O	2.18	0.43
1:C:358:ASN:O	1:C:359:GLN:CB	2.67	0.43
1:A:10:GLN:HE22	1:A:74:GLY:HA3	1.81	0.43
1:A:285:ALA:O	1:A:286:LEU:HD23	2.19	0.43
1:A:28:THR:O	1:A:32:HIS:HD2	2.01	0.43
1:A:91:ARG:HE	1:A:91:ARG:HB3	1.10	0.43
1:C:304:HIS:CE1	1:C:305:ILE:HG13	2.53	0.43
1:C:228:LEU:HD11	1:C:281:MET:HB3	1.99	0.43
1:A:162:TYR:CD2	1:A:299:GLN:HA	2.53	0.43
1:B:101:ARG:NH1	1:B:132:TYR:CE2	2.87	0.43
1:B:255:ARG:HB3	1:B:256:PHE:CD1	2.53	0.43
1:A:348:ILE:N	1:A:348:ILE:CD1	2.82	0.43
1:B:16:ALA:O	1:B:303:ARG:HD3	2.18	0.43
1:B:103:HIS:CE1	1:B:413:LYS:HD2	2.54	0.43
1:B:377:GLN:NE2	1:B:381:ASP:OD2	2.46	0.43
1:A:200:ALA:O	1:A:203:LEU:HD23	2.18	0.43
1:B:332:LEU:HA	1:B:351:ALA:O	2.18	0.43
1:C:211:PRO:HB3	1:C:242:VAL:CG2	2.47	0.43
1:B:338:ARG:NH1	1:B:344:TYR:HE1	2.15	0.42
1:A:70:HIS:HA	1:A:303:ARG:NE	2.33	0.42
1:B:148:PRO:HG3	1:B:359:GLN:O	2.19	0.42
1:C:416:THR:HG22	3:C:488:HOH:O	2.18	0.42
1:C:22:ALA:HA	1:C:25:VAL:CG1	2.49	0.42
1:C:182:THR:HA	1:C:289:LYS:HB3	2.01	0.42
1:C:303:ARG:HG3	1:C:303:ARG:HH11	1.83	0.42
1:A:95:ARG:NE	1:A:417:GLU:HG2	2.34	0.42
1:B:311:VAL:O	1:B:311:VAL:HG23	2.19	0.42
1:A:182:THR:N	1:A:289:LYS:HD3	2.34	0.42
1:A:222:PHE:CE2	1:A:281:MET:HE1	2.54	0.42
1:B:182:THR:HG21	1:B:291:HIS:CD2	2.54	0.42
1:B:205:GLY:HA3	1:B:211:PRO:O	2.20	0.42
1:B:285:ALA:O	1:B:286:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ALA:O	1:B:305:ILE:HD12	2.20	0.42
1:B:415:ARG:C	1:B:416:THR:HG23	2.44	0.42
1:C:275:ALA:N	1:C:276:PRO:CD	2.82	0.42
1:A:255:ARG:HB3	1:A:256:PHE:CD1	2.54	0.42
1:C:348:ILE:N	1:C:348:ILE:HD12	2.34	0.42
1:C:383:LEU:C	1:C:385:PRO:HD2	2.45	0.42
1:A:138:GLY:O	1:A:333:MET:HA	2.20	0.42
1:A:213:HIS:HD2	1:A:242:VAL:N	2.03	0.42
1:B:183:LYS:HE2	1:B:183:LYS:HB3	1.82	0.42
1:B:330:GLN:HG3	1:B:331:ALA:N	2.34	0.42
1:C:411:GLU:HA	3:C:456:HOH:O	2.20	0.42
1:A:95:ARG:CZ	1:A:414:LEU:HD23	2.49	0.42
1:A:143:VAL:HG22	1:A:159:VAL:CG1	2.49	0.42
1:A:186:ILE:HG23	1:A:243:VAL:CG2	2.50	0.42
1:A:205:GLY:HA3	1:A:211:PRO:O	2.20	0.42
1:B:22:ALA:HA	1:B:25:VAL:CG1	2.49	0.42
1:C:232:ASP:HB2	1:C:286:LEU:CD1	2.50	0.42
1:B:91:ARG:HE	1:B:91:ARG:HB3	1.10	0.41
1:B:202:GLY:HA3	1:B:375:ILE:CD1	2.47	0.41
1:C:117:GLN:HE22	1:C:138:GLY:HA3	1.84	0.41
1:C:338:ARG:NH1	1:C:344:TYR:HD1	2.18	0.41
1:C:50:LEU:O	1:C:417:GLU:CG	2.68	0.41
1:A:126:LEU:HD22	1:A:130:MET:SD	2.60	0.41
1:A:231:VAL:HG13	1:A:232:ASP:N	2.34	0.41
1:B:203:LEU:O	1:C:399:LEU:HD11	2.20	0.41
1:B:362:LYS:HE2	1:B:362:LYS:HB3	1.91	0.41
1:B:396:ASP:O	1:B:397:ASP:CB	2.67	0.41
1:C:205:GLY:HA3	1:C:211:PRO:O	2.21	0.41
1:C:213:HIS:HD2	1:C:242:VAL:N	2.06	0.41
1:B:188:GLU:HA	1:B:245:ALA:O	2.19	0.41
1:C:340:GLN:O	1:C:344:TYR:HA	2.20	0.41
1:B:17:VAL:HG22	1:B:155:GLY:HA2	2.01	0.41
1:B:182:THR:N	1:B:289:LYS:HD3	2.35	0.41
1:C:342:LYS:HB2	1:C:343:PRO:CD	2.40	0.41
1:A:417:GLU:OE2	1:A:418:PHE:O	2.39	0.41
1:B:136:CYS:N	1:B:330:GLN:HE22	2.07	0.41
1:A:135:THR:HA	1:A:330:GLN:NE2	2.35	0.41
1:A:341:ALA:O	1:A:342:LYS:C	2.63	0.41
1:B:117:GLN:HE22	1:B:138:GLY:HA3	1.86	0.41
1:B:278:LEU:O	1:B:281:MET:HB2	2.21	0.41
1:B:312:GLU:OE2	1:B:346:TRP:HZ2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ALA:H	1:C:276:PRO:CD	2.33	0.41
1:C:416:THR:O	1:C:417:GLU:CB	2.68	0.41
1:B:68:LEU:HA	1:B:71:THR:CG2	2.50	0.41
1:B:137:ILE:HG23	1:B:332:LEU:O	2.20	0.41
1:C:99:VAL:HG12	1:C:414:LEU:HD23	1.94	0.41
1:C:113:GLY:HA3	3:C:434:HOH:O	2.19	0.41
1:B:190:MET:HE3	3:B:504:HOH:O	2.20	0.41
1:B:293:ALA:HB2	1:C:296:ASP:HB3	2.02	0.41
1:C:145:ASN:HB2	1:C:156:PHE:CD2	2.56	0.41
1:C:203:LEU:N	1:C:203:LEU:HD22	2.36	0.41
1:C:222:PHE:HE2	1:C:281:MET:HE1	1.85	0.41
1:C:342:LYS:CB	1:C:343:PRO:CD	2.98	0.41
1:A:199:ALA:HB2	1:A:363:MET:HE1	2.03	0.41
1:B:15:THR:HG22	1:B:16:ALA:N	2.35	0.41
1:B:304:HIS:HE1	1:C:304:HIS:HE1	1.68	0.41
1:C:256:PHE:CD1	1:C:256:PHE:N	2.89	0.41
1:A:4:LYS:HB2	3:A:547:HOH:O	2.21	0.40
1:A:70:HIS:HB2	1:A:393:PRO:CB	2.50	0.40
1:A:142:THR:HG22	1:A:144:ASP:N	2.32	0.40
1:A:364:PRO:HG2	1:A:367:TYR:CD2	2.55	0.40
1:B:52:GLU:HG2	1:B:52:GLU:O	2.21	0.40
1:B:186:ILE:HG23	1:B:243:VAL:CG2	2.50	0.40
1:B:256:PHE:HA	3:B:427:HOH:O	2.21	0.40
1:A:143:VAL:HG11	1:A:190:MET:HE1	2.02	0.40
1:A:151:ASP:CG	1:A:338:ARG:HH21	2.30	0.40
1:B:70:HIS:HD2	1:B:401:ARG:O	2.03	0.40
1:B:175:LYS:HG2	1:B:240:TYR:CE2	2.56	0.40
1:B:193:HIS:HD2	3:B:455:HOH:O	2.03	0.40
1:B:390:GLU:HG2	1:B:392:PHE:CZ	2.57	0.40
1:C:183:LYS:HE2	1:C:183:LYS:HB3	1.82	0.40
1:A:365:ILE:C	1:A:367:TYR:N	2.79	0.40
1:A:232:ASP:O	1:A:235:VAL:HG22	2.21	0.40
1:A:404:LYS:HA	1:A:404:LYS:HD3	1.88	0.40
1:B:413:LYS:HE2	3:B:470:HOH:O	2.21	0.40
1:C:369:THR:HG23	1:C:374:GLY:C	2.47	0.40
1:C:382:TYR:C	1:C:385:PRO:HD2	2.46	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	384/420 (91%)	348 (91%)	30 (8%)	6 (2%)	7	14
1	B	384/420 (91%)	348 (91%)	29 (8%)	7 (2%)	6	12
1	C	384/420 (91%)	339 (88%)	37 (10%)	8 (2%)	5	9
All	All	1152/1260 (91%)	1035 (90%)	96 (8%)	21 (2%)	6	12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	PRO
1	A	412	LYS
1	B	343	PRO
1	B	344	TYR
1	B	359	GLN
1	C	343	PRO
1	C	359	GLN
1	C	417	GLU
1	A	403	ALA
1	B	416	THR
1	C	416	THR
1	A	344	TYR
1	A	414	LEU
1	A	417	GLU
1	B	397	ASP
1	B	417	GLU
1	C	344	TYR
1	C	369	THR
1	C	414	LEU
1	B	365	ILE
1	C	365	ILE

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	308/330 (93%)	269 (87%)	39 (13%)	4	9
1	B	308/330 (93%)	272 (88%)	36 (12%)	5	11
1	C	308/330 (93%)	272 (88%)	36 (12%)	5	11
All	All	924/990 (93%)	813 (88%)	111 (12%)	5	10

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	15	THR
1	A	25	VAL
1	A	43	ARG
1	A	46	ILE
1	A	50	LEU
1	A	71	THR
1	A	80	ARG
1	A	91	ARG
1	A	110	TYR
1	A	119	THR
1	A	126	LEU
1	A	135	THR
1	A	143	VAL
1	A	179	GLU
1	A	181	SER
1	A	182	THR
1	A	183	LYS
1	A	187	LEU
1	A	229	GLU
1	A	231	VAL
1	A	237	ASP
1	A	243	VAL
1	A	244	VAL
1	A	291	HIS
1	A	300	ARG

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Mol	Chain	Res	Type
1	A	305	ILE
1	A	311	VAL
1	A	323	GLU
1	A	326	LEU
1	A	343	PRO
1	A	355	GLU
1	A	360	GLU
1	A	361	LYS
1	A	371	ASN
1	A	409	LEU
1	A	413	LYS
1	A	414	LEU
1	A	417	GLU
1	B	4	LYS
1	B	15	THR
1	B	43	ARG
1	B	46	ILE
1	B	50	LEU
1	B	71	THR
1	B	80	ARG
1	B	91	ARG
1	B	110	TYR
1	B	119	THR
1	B	126	LEU
1	B	135	THR
1	B	143	VAL
1	B	159	VAL
1	B	179	GLU
1	B	181	SER
1	B	182	THR
1	B	183	LYS
1	B	187	LEU
1	B	229	GLU
1	B	231	VAL
1	B	237	ASP
1	B	243	VAL
1	B	244	VAL
1	B	292	TRP
1	B	300	ARG
1	B	305	ILE
1	B	311	VAL
1	B	323	GLU

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Mol	Chain	Res	Type
1	B	326	LEU
1	B	343	PRO
1	B	371	ASN
1	B	409	LEU
1	B	414	LEU
1	B	416	THR
1	B	417	GLU
1	C	15	THR
1	C	43	ARG
1	C	46	ILE
1	C	50	LEU
1	C	71	THR
1	C	80	ARG
1	C	91	ARG
1	C	119	THR
1	C	126	LEU
1	C	135	THR
1	C	143	VAL
1	C	179	GLU
1	C	181	SER
1	C	182	THR
1	C	183	LYS
1	C	187	LEU
1	C	229	GLU
1	C	231	VAL
1	C	237	ASP
1	C	243	VAL
1	C	244	VAL
1	C	291	HIS
1	C	300	ARG
1	C	305	ILE
1	C	343	PRO
1	C	355	GLU
1	C	359	GLN
1	C	370	ASP
1	C	371	ASN
1	C	408	GLN
1	C	409	LEU
1	C	411	GLU
1	C	414	LEU
1	C	415	ARG
1	C	416	THR

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Mol	Chain	Res	Type
1	C	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	27	GLN
1	A	32	HIS
1	A	44	ASN
1	A	66	GLN
1	A	70	HIS
1	A	111	ASN
1	A	117	GLN
1	A	206	GLN
1	A	213	HIS
1	A	250	GLN
1	A	284	GLN
1	A	291	HIS
1	A	330	GLN
1	A	352	ASN
1	A	371	ASN
1	A	408	GLN
1	B	10	GLN
1	B	32	HIS
1	B	44	ASN
1	B	66	GLN
1	B	70	HIS
1	B	103	HIS
1	B	111	ASN
1	B	117	GLN
1	B	206	GLN
1	B	213	HIS
1	B	284	GLN
1	B	330	GLN
1	B	352	ASN
1	B	371	ASN
1	B	408	GLN
1	C	10	GLN
1	C	32	HIS
1	C	44	ASN
1	C	66	GLN
1	C	70	HIS

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Mol	Chain	Res	Type
1	C	111	ASN
1	C	117	GLN
1	C	206	GLN
1	C	213	HIS
1	C	280	ASN
1	C	304	HIS
1	C	330	GLN
1	C	366	HIS
1	C	371	ASN
1	C	384	GLN
1	C	408	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	392/420 (93%)	0.59	29 (7%) 20 18	7, 27, 47, 62	2 (0%)
1	B	392/420 (93%)	0.98	51 (13%) 7 6	12, 33, 54, 66	2 (0%)
1	C	392/420 (93%)	1.09	63 (16%) 4 4	12, 34, 60, 67	2 (0%)
All	All	1176/1260 (93%)	0.89	143 (12%) 8 7	7, 32, 55, 67	6 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	THR	9.0
1	C	372	GLY	6.3
1	C	416	THR	6.3
1	B	418	PHE	5.5
1	B	91	ARG	5.4
1	A	416	THR	5.4
1	C	343	PRO	4.8
1	A	414	LEU	4.8
1	A	419	GLU	4.8
1	C	255	ARG	4.7
1	A	91	ARG	4.6
1	C	418	PHE	4.6
1	A	3	ILE	4.6
1	A	418	PHE	4.5
1	B	193	HIS	4.2
1	B	3	ILE	4.2
1	C	368	ILE	4.1
1	C	367	TYR	4.0
1	C	375	ILE	3.9
1	C	419	GLU	3.9
1	C	369	THR	3.9
1	C	420	LEU	3.8
1	B	132	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	414	LEU	3.7
1	A	193	HIS	3.7
1	C	342	LYS	3.6
1	B	420	LEU	3.6
1	C	362	LYS	3.5
1	A	420	LEU	3.5
1	C	371	ASN	3.5
1	C	250	GLN	3.5
1	B	341	ALA	3.4
1	C	359	GLN	3.4
1	C	403	ALA	3.3
1	C	248	GLY	3.3
1	A	251	TYR	3.3
1	B	415	ARG	3.3
1	C	370	ASP	3.2
1	C	192	ARG	3.2
1	C	252	GLU	3.2
1	B	273	GLY	3.2
1	C	256	PHE	3.2
1	C	376	THR	3.2
1	C	196	TRP	3.1
1	B	342	LYS	3.1
1	C	341	ALA	3.1
1	A	417	GLU	3.1
1	C	223	ASN	3.1
1	C	191	GLY	3.1
1	C	251	TYR	3.1
1	C	361	LYS	3.0
1	C	417	GLU	3.0
1	B	192	ARG	3.0
1	B	358	ASN	3.0
1	B	229	GLU	3.0
1	A	252	GLU	2.9
1	C	193	HIS	2.9
1	A	82	LYS	2.9
1	B	359	GLN	2.9
1	C	82	LYS	2.9
1	C	414	LEU	2.9
1	C	366	HIS	2.8
1	C	364	PRO	2.8
1	B	403	ALA	2.8
1	B	419	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	2.8
1	A	415	ARG	2.8
1	B	80	ARG	2.8
1	C	91	ARG	2.8
1	A	256	PHE	2.8
1	C	132	TYR	2.8
1	C	194	ALA	2.8
1	B	133	PRO	2.7
1	B	326	LEU	2.7
1	A	357	ALA	2.7
1	B	82	LYS	2.7
1	A	236	ARG	2.7
1	B	34	ASP	2.7
1	B	292	TRP	2.7
1	B	256	PHE	2.7
1	B	361	LYS	2.6
1	C	384	GLN	2.6
1	C	221	PRO	2.6
1	C	365	ILE	2.6
1	B	255	ARG	2.6
1	B	417	GLU	2.6
1	C	374	GLY	2.6
1	C	378	ASP	2.6
1	B	348	ILE	2.6
1	B	357	ALA	2.6
1	B	236	ARG	2.5
1	A	231	VAL	2.5
1	C	142	THR	2.5
1	A	343	PRO	2.5
1	B	104	ASP	2.5
1	C	292	TRP	2.5
1	A	80	ARG	2.5
1	C	206	GLN	2.4
1	C	274	VAL	2.4
1	B	4	LYS	2.4
1	C	3	ILE	2.4
1	B	251	TYR	2.4
1	B	207	SER	2.4
1	B	252	GLU	2.4
1	C	404	LYS	2.4
1	C	345	ARG	2.4
1	B	402	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	321	ALA	2.4
1	B	356	VAL	2.3
1	A	255	ARG	2.3
1	B	142	THR	2.3
1	C	360	GLU	2.3
1	A	66	GLN	2.3
1	B	66	GLN	2.3
1	B	37	GLY	2.2
1	C	66	GLN	2.2
1	B	375	ILE	2.2
1	B	33	PRO	2.2
1	B	223	ASN	2.2
1	C	326	LEU	2.2
1	C	379	CYS	2.2
1	B	343	PRO	2.2
1	B	235	VAL	2.2
1	A	371	ASN	2.2
1	A	206	GLN	2.2
1	B	340	GLN	2.1
1	C	231	VAL	2.1
1	B	284	GLN	2.1
1	C	335	THR	2.1
1	C	281	MET	2.1
1	C	249	ALA	2.1
1	A	192	ARG	2.1
1	A	235	VAL	2.1
1	C	236	ARG	2.1
1	B	31	LYS	2.1
1	C	347	SER	2.1
1	A	248	GLY	2.0
1	B	360	GLU	2.0
1	A	356	VAL	2.0
1	C	311	VAL	2.0
1	C	216	LEU	2.0
1	B	135	THR	2.0
1	A	132	TYR	2.0

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

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	NA	A	421	1/1	0.93	0.12	6,6,6,6	0
2	NA	B	421	1/1	0.94	0.09	1,1,1,1	0
2	NA	C	421	1/1	0.94	0.05	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.