Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:53 AM GMT

PDB ID	:	3K2Q
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

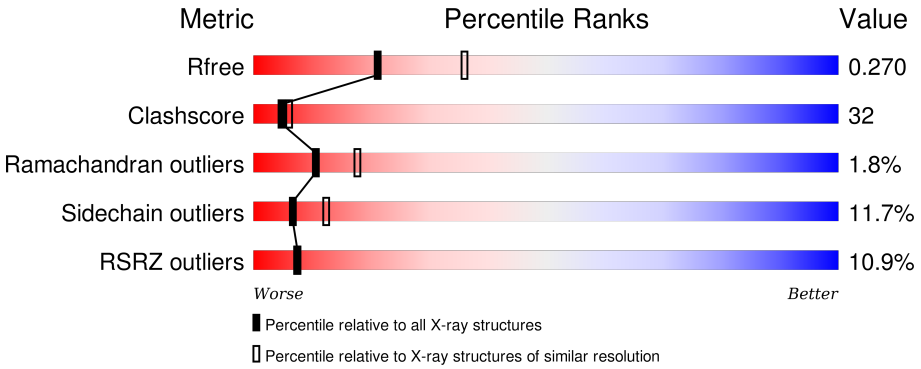
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5% 50% 37% 5% • 7%
1	B	420	10% 45% 42% 5% • 7%
1	C	420	16% 46% 40% 6% • 7%

2 Entry composition (i)

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 (three-letter code: NA) (formula: Na).

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

- Molecule 3 is water.

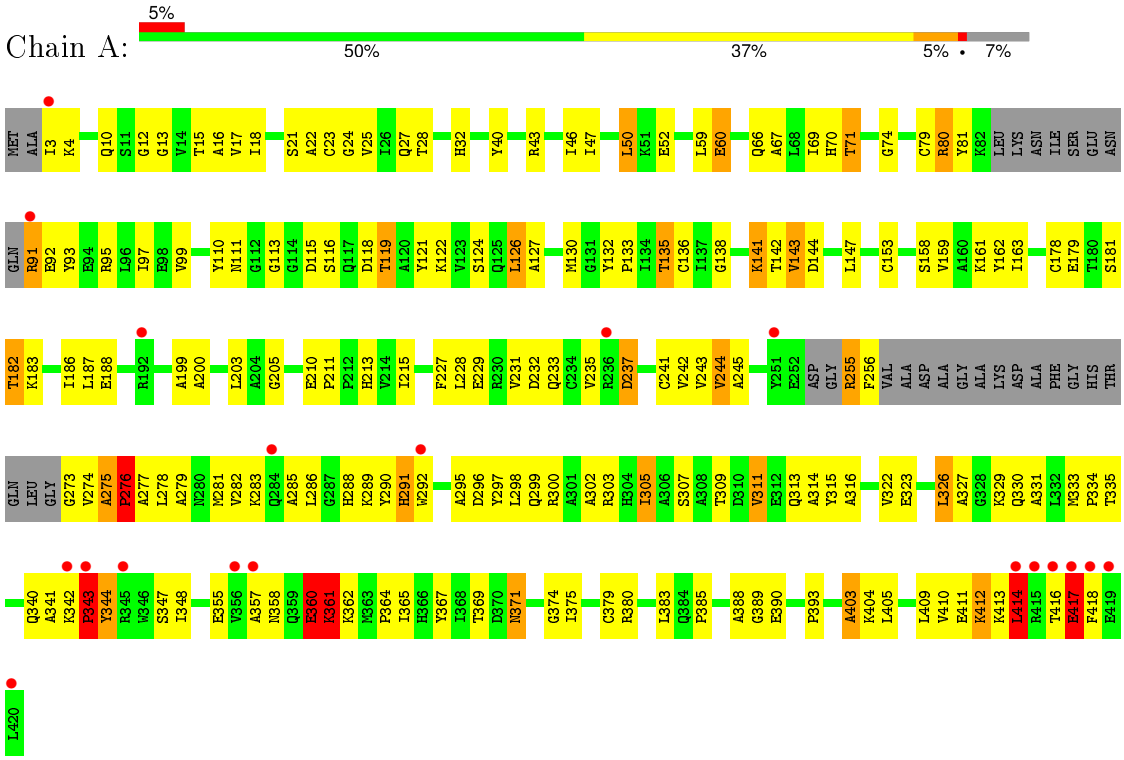
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	109	Total	O	0	0
			109	109		
3	C	119	Total	O	0	0
			119	119		

3 Residue-property plots (i)

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

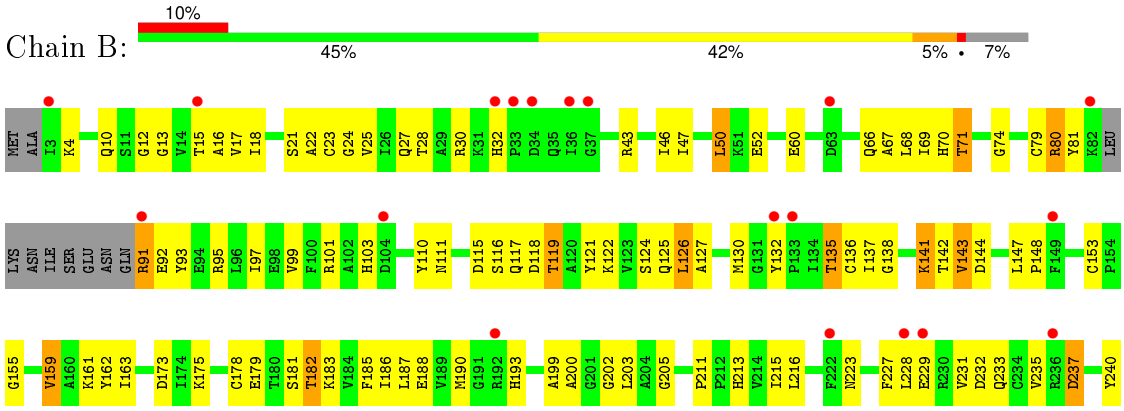
- Molecule 1: Pyrophosphate-dependent phosphofructokinase

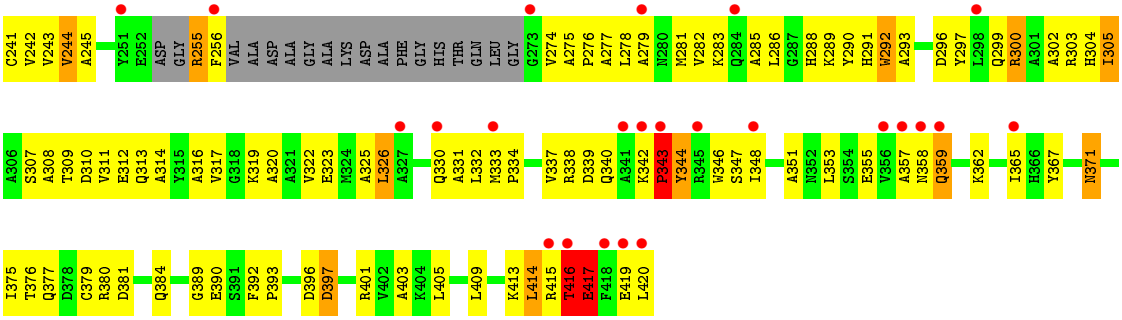
Chain A:



- Molecule 1: Pyrophosphate-dependent phosphofructokinase

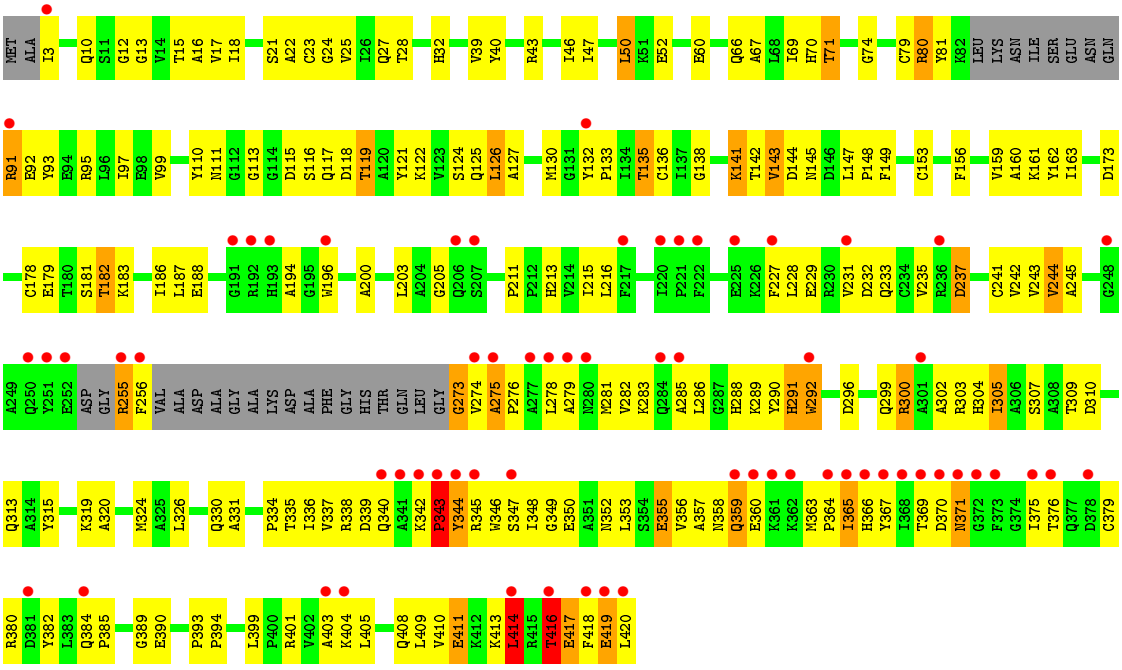
Chain B:





- Molecule 1: Pyrophosphate-dependent phosphofructokinase

Chain C:



4 Data and refinement statistics (i)

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 – 2.48	Depositor EDS
% Data completeness (in resolution range)	89.9 (44.70-2.50) 95.1 (44.70-2.48)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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	2082 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 97362 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.87	23/3073 (0.7%)	0.67	1/4157 (0.0%)
1	B	0.71	15/3073 (0.5%)	0.61	0/4157
1	C	0.49	2/3073 (0.1%)	0.62	0/4157
All	All	0.71	40/9219 (0.4%)	0.63	1/12471 (0.0%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	GLY	C-O	-16.46	0.97	1.23
1	B	420	LEU	C-OXT	15.37	1.52	1.23
1	B	277	ALA	CA-CB	-14.53	1.22	1.52
1	C	273	GLY	C-O	-12.65	1.03	1.23
1	A	278	LEU	C-O	-12.05	1.00	1.23
1	A	277	ALA	C-O	-9.04	1.06	1.23
1	A	361	LYS	CD-CE	-8.96	1.28	1.51
1	B	276	PRO	CG-CD	-8.74	1.21	1.50
1	A	274	VAL	C-O	-8.43	1.07	1.23
1	A	361	LYS	CE-NZ	-8.40	1.28	1.49
1	A	276	PRO	CB-CG	-7.97	1.10	1.50
1	A	276	PRO	CG-CD	-7.94	1.24	1.50
1	A	277	ALA	CA-CB	-7.86	1.35	1.52
1	B	276	PRO	CB-CG	-7.84	1.10	1.50
1	B	276	PRO	C-O	-7.44	1.08	1.23
1	B	275	ALA	C-O	-7.23	1.09	1.23
1	A	273	GLY	CA-C	-7.12	1.40	1.51
1	B	275	ALA	CA-CB	-7.02	1.37	1.52
1	B	277	ALA	C-O	-6.99	1.10	1.23
1	A	360	GLU	CD-OE2	-6.71	1.18	1.25
1	B	274	VAL	C-O	-6.60	1.10	1.23
1	A	278	LEU	CA-C	-6.38	1.36	1.52
1	A	361	LYS	CB-CG	-6.38	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	LYS	C-O	-6.37	1.11	1.23
1	A	276	PRO	C-O	-6.34	1.10	1.23
1	B	277	ALA	CA-C	-6.07	1.37	1.52
1	A	275	ALA	C-O	-5.98	1.11	1.23
1	B	276	PRO	CA-CB	-5.97	1.41	1.53
1	A	360	GLU	CD-OE1	-5.91	1.19	1.25
1	A	361	LYS	N-CA	-5.81	1.34	1.46
1	B	276	PRO	N-CD	-5.75	1.39	1.47
1	A	360	GLU	C-O	-5.74	1.12	1.23
1	A	275	ALA	CA-CB	-5.73	1.40	1.52
1	A	360	GLU	CB-CG	-5.61	1.41	1.52
1	C	275	ALA	CA-CB	-5.54	1.40	1.52
1	A	276	PRO	N-CD	-5.44	1.40	1.47
1	B	277	ALA	C-N	-5.35	1.21	1.34
1	B	275	ALA	N-CA	-5.17	1.36	1.46
1	B	276	PRO	N-CA	-5.14	1.38	1.47
1	A	278	LEU	CG-CD1	-5.04	1.33	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	LEU	CB-CG-CD2	5.63	120.57	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3010	0	2950	175	0
1	B	3010	0	2950	194	0
1	C	3010	0	2950	206	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	109	0	0	13	0
3	C	119	0	0	14	0
All	All	9397	0	8850	565	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 32.

All (565) 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: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
1:A:371:ASN:HD22	1:A:371:ASN:N	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:H	1:A:371:ASN:HD22	1.22	0.82
1:C:136:CYS:H	1:C:330:GLN:HE22	1.22	0.81
1:A:302:ALA:HB1	1:A:305:ILE:HD11	1.60	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:C:213:HIS:HD2	1:C:242:VAL:H	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:HIS:HD2	1:B: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:N	1:C:371:ASN:HD22	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:C:95:ARG:NH2	1:C:417:GLU:HB3	2.02	0.75
1:B:115:ASP:O	1:B:119:THR:HG22	1.86	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:H	1:B:371:ASN:ND2	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:B:213:HIS:CD2	1:B:241:CYS:HA	2.24	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:302:ALA:HB1	1:B:305:ILE:CD1	2.19	0.72
1:B:296:ASP:O	1:B:299:GLN:HG2	1.90	0.71
1:B:371:ASN:HD22	1:B:371:ASN:N	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:324:MET:CE	1:C:350:GLU:HG2	2.20	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:N	1:B:371:ASN:ND2	2.38	0.69
1:C:28:THR:HG21	1:C:319:LYS:CG	2.21	0.69
1:A:24:GLY:O	1:A:28:THR:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG21	1:A:288:HIS:NE2	2.08	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:HE3	1:C:350:GLU:HG2	1.75	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:B:136:CYS:H	1:B:330:GLN:NE2	1.91	0.69
1:A:13:GLY:H	1:A:80:ARG:NH2	1.91	0.69
1:C:13:GLY:H	1:C:80:ARG:HH21	1.39	0.69
1:B:358:ASN:O	1:B:359:GLN:HG2	1.93	0.68
1:B:235:VAL:HG21	1:B:288:HIS:NE2	2.07	0.68
1:B:118:ASP:OD1	1:B:122:LYS:HE2	1.93	0.68
1:A:142:THR:HG22	1:A:144:ASP:H	1.56	0.68
1:C:27:GLN:HE22	1:C:66:GLN:NE2	1.91	0.68
1:A:371:ASN:ND2	1:A:371:ASN:H	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:B:135:THR:HA	1:B:330:GLN:OE1	1.95	0.67
1:A:309:THR:HG23	1:A:388:ALA:O	1.94	0.67
1:A:330:GLN:HE21	1:A:331:ALA:N	1.91	0.67
1:C:274:VAL:O	1:C:274:VAL:HG12	1.95	0.67
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: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:136:CYS:H	1:A:330:GLN:NE2	1.93	0.66
1:A:118:ASP:HB2	1:A:357:ALA:HB2	1.77	0.66
1:B:67:ALA:O	1:B:71:THR:HG22	1.95	0.65
1:C:371:ASN:ND2	1:C:371:ASN:N	2.44	0.65
1:C:118:ASP:HB2	1:C:357:ALA:HB2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:342:LYS:CB	1:C:343:PRO:HD2	2.28	0.63
1:B:417:GLU:O	1:B:417:GLU:HG3	1.97	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: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:A:10:GLN:HE22	1:A:74:GLY:CA	2.12	0.62
1:B:27:GLN:HE22	1:B:66:GLN:HE21	1.48	0.62
1:B:10:GLN:HE22	1:B:74:GLY:CA	2.12	0.62
1:A:416:THR:HG22	1:A:417:GLU:N	2.13	0.62
1:A:342:LYS:O	1:A:343:PRO:C	2.38	0.62
1:C:10:GLN:HE22	1:C:74:GLY:CA	2.12	0.61
1:C:136:CYS:N	1:C:330:GLN:HE22	1.94	0.61
1:C:211:PRO:HB3	1:C:242:VAL:HG21	1.82	0.61
1:B:232:ASP:HB2	1:B:286:LEU:HD13	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:B:99:VAL:HG12	1:B:414:LEU:HD22	1.83	0.61
1:A:91:ARG:HG3	1:A:92:GLU:H	1.65	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:A:322:VAL:O	1:A:326:LEU:HD22	2.01	0.60
1:C:91:ARG:HG3	1:C:92:GLU:H	1.66	0.60
1:B:396:ASP:O	1:B:397:ASP:HB2	2.01	0.60
1:B:91:ARG:HG3	1:B:92:GLU:H	1.66	0.60
1:C:358:ASN:O	1:C:359:GLN:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:342:LYS:O	1:C:343:PRO:C	2.39	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:47:ILE:HD11	1:C:81:TYR:CG	2.38	0.59
1:C:27:GLN:HE22	1:C:66:GLN:HE21	1.48	0.59
1:C:382:TYR:O	1:C:385:PRO:HD2	2.03	0.58
1:C:182:THR:HG21	1:C:291:HIS:CD2	2.38	0.58
1:A:403:ALA:O	1:A:404:LYS:HB2	2.02	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:342:LYS:HB2	1:B:343:PRO:CD	2.23	0.58
1:B:279:ALA:HB1	1:B:290:TYR:CD2	2.38	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: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:329:LYS:NZ	1:B:340:GLN:HG3	2.20	0.57
1:A:60:GLU:CG	1:A:405:LEU:HD22	2.32	0.57
1:A:18:ILE:HD12	1:A:141:LYS:HG3	1.86	0.57
1:A:295:ALA:O	1:A:298:LEU:HB2	2.04	0.57
1:C:50:LEU:O	1:C:417:GLU:HG2	2.05	0.57
1:A:21:SER:O	1:A:25:VAL:HG12	2.04	0.57
1:C:156:PHE:CE2	1:C:196:TRP:HB3	2.40	0.56
1:A:335:THR:O	1:A:348:ILE:HA	2.05	0.56
1:C:145:ASN:HA	1:C:153:CYS:SG	2.45	0.56
1:C:3:ILE:O	1:C:3:ILE:HG23	2.06	0.56
1:C:15:THR:CG2	1:C:16:ALA:N	2.69	0.56
1:B:342:LYS:O	1:B:343:PRO:C	2.44	0.56
1:A:375:ILE:HG13	1:A:379:CYS:HB3	1.86	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:200:ALA:HA	1:B:203:LEU:HD23	1.88	0.56
1:B:18:ILE:HD12	1:B:141:LYS:HG3	1.88	0.56
1:B:211:PRO:HB3	1:B:242:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HD12	1:A:305:ILE:H	1.71	0.55
1:C:18:ILE:HD12	1:C:141:LYS:HG3	1.87	0.55
1:A:147:LEU:HB2	1:A:153:CYS:SG	2.45	0.55
1:B:337:VAL:HG22	1:B:347:SER:O	2.07	0.55
1:B:141:LYS:C	1:B:141:LYS:HD2	2.27	0.55
1:B:380:ARG:NH1	1:B:380:ARG:HG3	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:C:320:ALA:HB1	1:C:348:ILE:HG21	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: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:59:LEU:HB3	3:A:483:HOH:O	2.08	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:338:ARG:NH1	1:B:344:TYR:CE1	2.75	0.54
1:B:199:ALA:O	1:B:375:ILE:CD1	2.55	0.54
1:B:340:GLN:HG2	1:B:342:LYS:CG	2.36	0.54
1:B:147:LEU:HB2	1:B:153:CYS:SG	2.48	0.54
1:C:355:GLU:HB3	3:C:515:HOH:O	2.08	0.54
1:C:142:THR:HA	3:C:502:HOH:O	2.08	0.54
1:A:10:GLN:NE2	3:A:422:HOH:O	2.40	0.54
1:C:116:SER:O	1:C:119:THR:HG23	2.07	0.54
1:B:358:ASN:O	1:B:359:GLN:CG	2.56	0.54
1:C:127:ALA:HB1	1:C:132:TYR:O	2.05	0.54
1:C:419:GLU:CG	1:C:420:LEU:N	2.53	0.53
1:C:135:THR:HA	1:C:330:GLN:HE22	1.74	0.53
1:A:116:SER:O	1:A:119:THR:HG23	2.09	0.53
1:A:275:ALA:HB3	1:A:276:PRO:CD	2.39	0.53
1:B:300:ARG:CD	1:C:173:ASP:OD2	2.57	0.53
1:C:95:ARG:CZ	1:C:417:GLU:CB	2.86	0.53
1:A:371:ASN:ND2	1:A:371:ASN:N	2.45	0.53
1:C:338:ARG:NH1	1:C:344:TYR:CD1	2.77	0.53
1:A:291:HIS:HB2	3:A:424:HOH:O	2.08	0.53
1:B:127:ALA:HB1	1:B:132:TYR:O	2.09	0.53
1:A:211:PRO:HB3	1:A:242:VAL:HG21	1.89	0.53
1:C:143:VAL:HG22	1:C:159:VAL:CG1	2.37	0.53
1:B:307:SER:HB3	1:B:310:ASP:CB	2.39	0.53
1:C:178:CYS:O	1:C:183:LYS:HE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:HD2	1:A:141:LYS:C	2.30	0.53
1:A:93:TYR:HB3	1:A:126:LEU:HD12	1.91	0.53
1:C:135:THR:HA	1:C:330:GLN:NE2	2.24	0.52
1:B:305:ILE:N	1:B:305:ILE:HD12	2.21	0.52
1:B:15:THR:CG2	1:B:16:ALA:N	2.72	0.52
1:A:348:ILE:HD12	1:A:348:ILE:N	2.23	0.52
1:A:143:VAL:HG22	1:A:159:VAL:HG11	1.91	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:C:324:MET:HE2	1:C:350:GLU:HG2	1.90	0.52
1:C:274:VAL:CG1	1:C:274:VAL:O	2.56	0.52
1:B:186:ILE:O	1:B:292:TRP:HA	2.09	0.52
1:A:127:ALA:HB1	1:A:132:TYR:O	2.09	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: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:C:141:LYS:C	1:C:141:LYS:HD2	2.31	0.51
1:B:70:HIS:HB2	1:B:393:PRO:CB	2.37	0.51
1:C:231:VAL:HG13	1:C:232:ASP:H	1.76	0.51
1:B:23:CYS:SG	1:B:69:ILE:CG2	2.99	0.51
1:A:40:TYR:CE1	1:A:410:VAL:HG21	2.46	0.51
1:C:182:THR:HG21	1:C:291:HIS:HD2	1.76	0.51
1:A:4:LYS:NZ	3:A:455:HOH:O	2.44	0.51
1:A:199:ALA:HB1	1:A:375:ILE:HD11	1.93	0.51
1:C:330:GLN:HE21	1:C:331:ALA:H	1.59	0.51
1:C:320:ALA:CB	1:C:348:ILE:HG21	2.41	0.51
1:A:95:ARG:CZ	1:A:417:GLU:CB	2.88	0.51
1:B:95:ARG:HE	1:B:417:GLU:HG2	1.74	0.51
1:A:10:GLN:HE22	1:A:74:GLY:HA2	1.75	0.51
1:A:316:ALA:HB1	1:A:348:ILE:HD11	1.93	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:340:GLN:O	1:A:344:TYR:HA	2.10	0.50
1:A:291:HIS:N	3:A:424:HOH:O	2.44	0.50
1:C:337:VAL:O	1:C:346:TRP:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:186:ILE:HG12	1:C:243:VAL:HG22	1.92	0.50
1:B:21:SER:O	1:B:25:VAL:HG12	2.11	0.50
1:C:255:ARG:HB3	1:C:256:PHE:HD1	1.75	0.50
1:C:419:GLU:CG	1:C:420:LEU:H	2.20	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:273:GLY:O	1:C:276:PRO:HD2	2.11	0.50
1:B:93:TYR:HB3	1:B:126:LEU:HD12	1.93	0.50
1:C:95:ARG:CZ	1:C:417:GLU:HB3	2.42	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:A:182:THR:HG21	1:A:291:HIS:HD2	1.75	0.50
1:B:231:VAL:HG13	1:B:232:ASP:H	1.77	0.50
1:A:91:ARG:CG	1:A:92:GLU:H	2.24	0.49
1:A:417:GLU:O	1:A:417:GLU:HG3	2.10	0.49
1:C:147:LEU:HB2	1:C:153:CYS:SG	2.53	0.49
1:C:121:TYR:O	1:C:124:SER:HB3	2.12	0.49
1:A:255:ARG:HB3	1:A:256:PHE:HD1	1.77	0.49
1:B:213:HIS:CD2	1:B:242:VAL:H	2.18	0.49
1:B:125:GLN:NE2	3:B:529:HOH:O	2.44	0.49
1:C:342:LYS:O	1:C:344:TYR:N	2.45	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:360:GLU:HB3	3:C:506:HOH:O	2.11	0.49
1:C:10:GLN:HE22	1:C:74:GLY:HA2	1.77	0.49
1:B:316:ALA:HB1	1:B:348:ILE:HD11	1.94	0.49
1:A:23:CYS:SG	1:A:69:ILE:CG2	3.00	0.49
1:B:357:ALA:O	1:B:358:ASN:HB2	2.12	0.49
1:B:216:LEU:HA	3:B:517:HOH:O	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:279:ALA:O	1:C:282:VAL:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:TYR:HD2	1:C:163:ILE:HD12	1.77	0.49
1:C:23:CYS:SG	1:C:69:ILE:CG2	3.01	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:C:384:GLN:HG3	1:C:385:PRO:HD3	1.94	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:A:365:ILE:C	1:A:367:TYR:H	2.16	0.49
1:C:159:VAL:CG2	1:C:160:ALA:N	2.76	0.48
1:A:380:ARG:HD3	3:A:470:HOH:O	2.11	0.48
1:A:158:SER:HB3	3:A:453:HOH:O	2.13	0.48
1:A:162:TYR:HD2	1:A:163:ILE:HD12	1.77	0.48
1:C:363:MET:HB2	3:C:432:HOH:O	2.12	0.48
1:C:10:GLN:HE22	1:C:74:GLY:HA3	1.79	0.48
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.94	0.48
1:C:40:TYR:CE1	1:C:410:VAL:HG21	2.48	0.48
1:A:411:GLU:O	1:A:412:LYS:O	2.30	0.48
1:C:307:SER:HB3	1:C:310:ASP:HB2	1.95	0.48
1:C:394:PRO:HG3	1:C:401:ARG:NH1	2.28	0.48
1:C:28:THR:CG2	1:C:319:LYS:HG3	2.27	0.48
1:B:119:THR:HG21	3:B:422:HOH:O	2.12	0.48
1:A:91:ARG:HG2	3:A:423:HOH:O	2.12	0.48
1:B:255:ARG:HB3	1:B:256:PHE:HD1	1.78	0.48
1:B:242:VAL:O	1:B:242:VAL:HG23	2.13	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:C:371:ASN:ND2	1:C:371:ASN:H	2.09	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: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:B:4:LYS:HB2	1:B:4:LYS:NZ	2.29	0.48
1:C:133:PRO:HA	3:C:441:HOH:O	2.12	0.48
1:A:279:ALA:O	1:A:282:VAL:HG22	2.13	0.48
1:A:126:LEU:CD2	1:A:130:MET:HG3	2.43	0.48
1:B:308:ALA:HB2	1:B:390:GLU:O	2.14	0.48
1:A:215:ILE:HG12	1:A:244:VAL:CG1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:VAL:HG23	3:C:462:HOH:O	2.13	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:A:161:LYS:NZ	1:A:390:GLU:HG3	2.30	0.47
1:C:24:GLY:HA2	1:C:315:TYR:CE1	2.49	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:C:215:ILE:HG12	1:C:244:VAL:CG1	2.44	0.47
1:C:242:VAL:O	1:C:242:VAL:HG23	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: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:A:47:ILE:HG12	1:A:79:CYS:SG	2.55	0.47
1:A:21:SER:HA	1:A:314:ALA:O	2.15	0.47
1:C:227:PHE:O	1:C:231:VAL:HG12	2.14	0.47
1:B:322:VAL:O	1:B:325:ALA:HB3	2.15	0.47
1:C:15:THR:CG2	1:C:17:VAL:H	2.08	0.47
1:B:28:THR:HG21	1:B:319:LYS:HG3	1.97	0.47
1:A:126:LEU:HD22	1:A:130:MET:HG3	1.97	0.47
1:A:213:HIS:CD2	1:A:242:VAL:H	2.16	0.46
1:B:355:GLU:C	1:B:357:ALA:N	2.68	0.46
1:A:290:TYR:C	3:A:424:HOH:O	2.54	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:C:200:ALA:O	1:C:203:LEU:HD23	2.15	0.46
1:A:364:PRO:O	1:A:367:TYR:HB2	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:C:285:ALA:O	1:C:286:LEU:HD23	2.16	0.46
1:B:126:LEU:HD22	1:B:130:MET:HG3	1.98	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: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:B:95:ARG:CZ	1:B:417:GLU:CB	2.91	0.46
1:B:60:GLU:CG	1:B:405:LEU:HD22	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HB3	1:C:91:ARG:HE	1.10	0.46
1:A:242:VAL:O	1:A:242:VAL:HG23	2.15	0.46
1:C:12:GLY:HA2	1:C:80:ARG:HE	1.80	0.46
1:B:228:LEU:HD11	1:B:281:MET:HB3	1.97	0.46
1:C:337:VAL:CG2	1:C:347:SER:OG	2.64	0.46
1:A:121:TYR:O	1:A:124:SER:HB3	2.16	0.46
1:A:375:ILE:CG1	1:A:379:CYS:SG	3.04	0.46
1:A:12:GLY:HA2	1:A:80:ARG:HE	1.81	0.46
1:A:307:SER:O	1:A:311:VAL:HG13	2.16	0.45
1:A:383:LEU:C	1:A:385:PRO:HD2	2.37	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:C:213:HIS:CD2	1:C:242:VAL:H	2.18	0.45
1:B:367:TYR:O	1:B:376:THR:HG23	2.16	0.45
1:B:70:HIS:CD2	1:B:401:ARG:O	2.70	0.45
1:C:367:TYR:C	1:C:376:THR:HG23	2.37	0.45
1:C:292:TRP:C	1:C:292:TRP:CD1	2.89	0.45
1:C:231:VAL:HG13	1:C:232:ASP:N	2.32	0.45
1:C:15:THR:HG22	1:C:16:ALA:N	2.31	0.45
1:A:161:LYS:HE3	1:A:389:GLY:O	2.16	0.45
1:C:380:ARG:HG3	1:C:380:ARG:HH11	1.82	0.45
1:A:22:ALA:HA	1:A:25:VAL:CG1	2.47	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:338:ARG:NH1	1:B:344:TYR:CD1	2.83	0.44
1:A:341:ALA:C	1:A:342:LYS:O	2.54	0.44
1:C:161:LYS:HZ2	1:C:390:GLU:HG3	1.82	0.44
1:C:313:GLN:HB3	1:C:336:ILE:CD1	2.48	0.44
1:B:314:ALA:O	1:B:317:VAL:HG22	2.17	0.44
1:B:143:VAL:CG2	1:B:159:VAL:HG11	2.45	0.44
1:B:28:THR:O	1:B:32:HIS:HD2	2.00	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:A:52:GLU:OE2	1:A:414:LEU:HB2	2.18	0.44
1:B:213:HIS:HD2	1:B:242:VAL:N	2.05	0.44
1:B:50:LEU:O	1:B:417:GLU:HG2	2.17	0.44
1:C:118:ASP:HB2	1:C:357:ALA:CB	2.46	0.44
1:B:81:TYR:OH	1:B:419:GLU:HB2	2.18	0.44
1:A:329:LYS:HZ3	1:B:340:GLN:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ASN:O	1:C:356:VAL:HG23	2.18	0.44
1:C:28:THR:O	1:C:32:HIS:HD2	2.01	0.44
1:B:331:ALA:O	1:B:353:LEU:HG	2.18	0.44
1:C:143:VAL:CG2	1:C:159:VAL:HG11	2.46	0.44
1:C:70:HIS:HA	1:C:303:ARG:NH2	2.33	0.44
1:B:231:VAL:HG13	1:B:232:ASP:N	2.33	0.44
1:B:47:ILE:HG12	1:B:79:CYS:SG	2.57	0.44
1:B:326:LEU:CD1	1:B:326:LEU:N	2.80	0.44
1:C:364:PRO:O	1:C:367:TYR:HB2	2.18	0.44
1:C:91:ARG:N	3:C:436:HOH:O	2.51	0.44
1:B:97:ILE:HD13	1:B:127:ALA:HA	1.99	0.43
1:A:97:ILE:HD13	1:A:127:ALA:HA	2.00	0.43
1:C:186:ILE:HG23	1:C:243:VAL:CG2	2.48	0.43
1:B:296:ASP:CG	1:B:297:TYR:H	2.21	0.43
1:B:161:LYS:HE3	1:B:389:GLY:O	2.18	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:A:182:THR:HA	1:A:289:LYS:HB3	2.00	0.43
1:C:403:ALA:O	1:C:404:LYS:HB2	2.18	0.43
1:C:358:ASN:O	1:C:359:GLN:CB	2.67	0.43
1:B:182:THR:HA	1:B:289:LYS:HB3	2.00	0.43
1:A:188:GLU:HA	1:A:245:ALA:O	2.18	0.43
1:A:369:THR:HG23	1:A:374:GLY:C	2.38	0.43
1:C:188:GLU:HA	1:C:245:ALA:O	2.18	0.43
1:A:285:ALA:O	1:A:286:LEU:HD23	2.19	0.43
1:A:10:GLN:HE22	1:A:74:GLY:HA3	1.81	0.43
1:C:304:HIS:CE1	1:C:305:ILE:HG13	2.53	0.43
1:A:28:THR:O	1:A:32:HIS:HD2	2.01	0.43
1:A:91:ARG:HB3	1:A:91:ARG:HE	1.10	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:B:16:ALA:O	1:B:303:ARG:HD3	2.18	0.43
1:A:296:ASP:CG	1:A:297:TYR:H	2.22	0.43
1:A:348:ILE:CD1	1:A:348:ILE:N	2.82	0.43
1:B:377:GLN:NE2	1:B:381:ASP:OD2	2.46	0.43
1:B:103:HIS:CE1	1:B:413:LYS:HD2	2.54	0.43
1:C:211:PRO:HB3	1:C:242:VAL:CG2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ARG:NH1	1:B:344:TYR:HE1	2.15	0.42
1:C:416:THR:HG22	3:C:488:HOH:O	2.18	0.42
1:B:148:PRO:HG3	1:B:359:GLN:O	2.19	0.42
1:A:70:HIS:HA	1:A:303:ARG:NE	2.33	0.42
1:C:182:THR:HA	1:C:289:LYS:HB3	2.01	0.42
1:C:303:ARG:HH11	1:C:303:ARG:HG3	1.83	0.42
1:C:22:ALA:HA	1:C:25:VAL:CG1	2.49	0.42
1:A:95:ARG:NE	1:A:417:GLU:HG2	2.34	0.42
1:B:311:VAL:HG23	1:B:311:VAL:O	2.19	0.42
1:B:205:GLY:HA3	1:B:211:PRO:O	2.20	0.42
1:B:302:ALA:O	1:B:305:ILE:HD12	2.20	0.42
1:A:182:THR:N	1:A:289:LYS:HD3	2.34	0.42
1:B:285:ALA:O	1:B:286:LEU:HD23	2.20	0.42
1:B:182:THR:HG21	1:B:291:HIS:CD2	2.54	0.42
1:C:275:ALA:N	1:C:276:PRO:CD	2.82	0.42
1:C:348:ILE:N	1:C:348:ILE:HD12	2.34	0.42
1:A:255:ARG:HB3	1:A:256:PHE:CD1	2.54	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:330:GLN:HG3	1:B:331:ALA:N	2.34	0.42
1:C:365:ILE:C	1:C:367:TYR:H	2.23	0.42
1:B:183:LYS:HE2	1:B:183:LYS:HB3	1.82	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:205:GLY:HA3	1:A:211:PRO:O	2.20	0.42
1:C:232:ASP:HB2	1:C:286:LEU:CD1	2.50	0.42
1:A:186:ILE:HG23	1:A:243:VAL:CG2	2.50	0.42
1:A:143:VAL:HG22	1:A:159:VAL:CG1	2.49	0.42
1:B:22:ALA:HA	1:B:25:VAL:CG1	2.49	0.42
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:B:202:GLY:HA3	1:B:375:ILE:CD1	2.47	0.41
1:B:91:ARG:HE	1:B:91:ARG:HB3	1.10	0.41
1:B:190:MET:HE3	3:B:504:HOH:O	2.19	0.41
1:C:50:LEU:O	1:C:417:GLU:CG	2.68	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: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:396:ASP:O	1:B:397:ASP:CB	2.67	0.41
1:A:126:LEU:HD22	1:A:130:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:HE2	1:B:362:LYS:HB3	1.91	0.41
1:C:340:GLN:O	1:C:344:TYR:HA	2.20	0.41
1:B:188:GLU:HA	1:B:245:ALA:O	2.19	0.41
1:B:17:VAL:HG22	1:B:155:GLY:HA2	2.01	0.41
1:C:342:LYS:HB2	1:C:343:PRO:CD	2.40	0.41
1:B:182:THR:N	1:B:289:LYS:HD3	2.35	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:B:117:GLN:HE22	1:B:138:GLY:HA3	1.86	0.41
1:C:416:THR:O	1:C:417:GLU:CB	2.68	0.41
1:B:278:LEU:O	1:B:281:MET:HB2	2.21	0.41
1:C:275:ALA:H	1:C:276:PRO:CD	2.33	0.41
1:B:312:GLU:OE2	1:B:346:TRP:HZ2	2.03	0.41
1:C:99:VAL:HG12	1:C:414:LEU:HD23	1.94	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:113:GLY:HA3	3:C:434:HOH:O	2.19	0.41
1:C:342:LYS:CB	1:C:343:PRO:CD	2.98	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:HD22	1:C:203:LEU:N	2.36	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:N	1:C:256:PHE:CD1	2.89	0.41
1:A:361:LYS:O	1:A:361:LYS:CG	2.67	0.41
1:B:52:GLU:HG2	1:B:52:GLU:O	2.21	0.40
1:A:142:THR:HG22	1:A:144:ASP:N	2.32	0.40
1:A:70:HIS:HB2	1:A:393:PRO:CB	2.50	0.40
1:B:186:ILE:HG23	1:B:243:VAL:CG2	2.50	0.40
1:A:4:LYS:HB2	3:A:547:HOH:O	2.21	0.40
1:A:364:PRO:HG2	1:A:367:TYR:CD2	2.55	0.40
1:B:256:PHE:HA	3:B:427:HOH:O	2.21	0.40
1:B:70:HIS:HD2	1:B:401:ARG:O	2.03	0.40
1:C:183:LYS:HE2	1:C:183:LYS:HB3	1.82	0.40
1:B:390:GLU:HG2	1:B:392:PHE:CZ	2.57	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:331:ALA:C	1:B:353:LEU:HG	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LYS:HE2	3:B:470:HOH:O	2.21	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	384/420 (91%)	348 (91%)	30 (8%)	6 (2%)	12 21
1	B	384/420 (91%)	348 (91%)	29 (8%)	7 (2%)	11 18
1	C	384/420 (91%)	339 (88%)	37 (10%)	8 (2%)	9 14
All	All	1152/1260 (91%)	1035 (90%)	96 (8%)	21 (2%)	11 18

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

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Mol	Chain	Res	Type
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	308/330 (93%)	268 (87%)	40 (13%)	5 9
1	B	308/330 (93%)	275 (89%)	33 (11%)	8 15
1	C	308/330 (93%)	273 (89%)	35 (11%)	7 13
All	All	924/990 (93%)	816 (88%)	108 (12%)	7 12

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	43	ARG
1	A	46	ILE
1	A	50	LEU
1	A	60	GLU
1	A	71	THR
1	A	80	ARG
1	A	91	ARG
1	A	110	TYR
1	A	111	ASN
1	A	119	THR
1	A	126	LEU
1	A	135	THR
1	A	141	LYS
1	A	143	VAL
1	A	179	GLU
1	A	181	SER

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Mol	Chain	Res	Type
1	A	182	THR
1	A	187	LEU
1	A	229	GLU
1	A	237	ASP
1	A	244	VAL
1	A	255	ARG
1	A	276	PRO
1	A	291	HIS
1	A	292	TRP
1	A	300	ARG
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	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	111	ASN
1	B	119	THR
1	B	126	LEU
1	B	135	THR
1	B	141	LYS
1	B	143	VAL
1	B	159	VAL
1	B	179	GLU
1	B	181	SER
1	B	182	THR
1	B	187	LEU
1	B	229	GLU

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Mol	Chain	Res	Type
1	B	237	ASP
1	B	244	VAL
1	B	255	ARG
1	B	292	TRP
1	B	300	ARG
1	B	305	ILE
1	B	323	GLU
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	43	ARG
1	C	46	ILE
1	C	50	LEU
1	C	71	THR
1	C	80	ARG
1	C	91	ARG
1	C	110	TYR
1	C	111	ASN
1	C	119	THR
1	C	126	LEU
1	C	135	THR
1	C	141	LYS
1	C	143	VAL
1	C	179	GLU
1	C	181	SER
1	C	182	THR
1	C	187	LEU
1	C	229	GLU
1	C	237	ASP
1	C	244	VAL
1	C	255	ARG
1	C	291	HIS
1	C	292	TRP
1	C	300	ARG
1	C	305	ILE
1	C	343	PRO
1	C	355	GLU
1	C	370	ASP

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Mol	Chain	Res	Type
1	C	371	ASN
1	C	408	GLN
1	C	409	LEU
1	C	411	GLU
1	C	414	LEU
1	C	416	THR
1	C	419	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	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	284	GLN
1	A	291	HIS
1	A	330	GLN
1	A	352	ASN
1	A	371	ASN
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	C	10	GLN
1	C	32	HIS
1	C	44	ASN

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Mol	Chain	Res	Type
1	C	66	GLN
1	C	70	HIS
1	C	111	ASN
1	C	117	GLN
1	C	213	HIS
1	C	284	GLN
1	C	304	HIS
1	C	330	GLN
1	C	366	HIS
1	C	371	ASN
1	C	384	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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%)	0.37	19 (4%) 34 39	7, 27, 47, 62	2 (0%)
1	B	392/420 (93%)	0.81	43 (10%) 7 7	12, 33, 54, 66	2 (0%)
1	C	392/420 (93%)	1.03	66 (16%) 2 2	12, 34, 60, 67	2 (0%)
All	All	1176/1260 (93%)	0.74	128 (10%) 7 7	7, 32, 55, 67	6 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	372	GLY	10.3
1	B	416	THR	7.8
1	C	369	THR	6.0
1	B	91	ARG	6.0
1	C	416	THR	5.8
1	C	418	PHE	5.8
1	B	418	PHE	5.7
1	A	418	PHE	5.6
1	C	251	TYR	5.5
1	C	367	TYR	5.4
1	C	362	LYS	5.0
1	A	416	THR	4.7
1	B	3	ILE	4.6
1	C	368	ILE	4.6
1	C	373	PHE	4.5
1	C	255	ARG	4.4
1	C	252	GLU	4.4
1	C	359	GLN	4.4
1	A	91	ARG	4.2
1	C	345	ARG	4.1
1	A	420	LEU	4.1
1	C	342	LYS	4.1
1	A	3	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	341	ALA	4.0
1	C	192	ARG	4.0
1	C	375	ILE	4.0
1	C	343	PRO	4.0
1	B	343	PRO	4.0
1	B	236	ARG	4.0
1	B	420	LEU	3.9
1	C	236	ARG	3.8
1	B	132	TYR	3.6
1	B	359	GLN	3.5
1	C	365	ILE	3.4
1	C	222	PHE	3.3
1	C	3	ILE	3.3
1	C	371	ASN	3.3
1	C	420	LEU	3.2
1	C	341	ALA	3.2
1	B	342	LYS	3.1
1	C	250	GLN	3.1
1	B	192	ARG	3.0
1	C	248	GLY	3.0
1	C	279	ALA	3.0
1	A	414	LEU	3.0
1	C	284	GLN	3.0
1	C	378	ASP	2.9
1	B	419	GLU	2.9
1	C	191	GLY	2.9
1	C	196	TRP	2.9
1	B	357	ALA	2.9
1	C	364	PRO	2.9
1	B	358	ASN	2.8
1	B	279	ALA	2.8
1	C	360	GLU	2.7
1	B	298	LEU	2.7
1	C	285	ALA	2.7
1	A	284	GLN	2.7
1	C	340	GLN	2.7
1	B	284	GLN	2.7
1	B	345	ARG	2.7
1	C	366	HIS	2.6
1	C	221	PRO	2.6
1	C	370	ASP	2.6
1	C	344	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	33	PRO	2.6
1	B	34	ASP	2.6
1	B	256	PHE	2.6
1	B	251	TYR	2.6
1	C	403	ALA	2.6
1	B	222	PHE	2.5
1	C	206	GLN	2.5
1	C	278	LEU	2.5
1	B	229	GLU	2.5
1	C	193	HIS	2.5
1	C	132	TYR	2.5
1	C	301	ALA	2.5
1	C	414	LEU	2.5
1	A	236	ARG	2.4
1	B	327	ALA	2.4
1	A	192	ARG	2.4
1	B	104	ASP	2.4
1	C	376	THR	2.4
1	A	357	ALA	2.4
1	B	32	HIS	2.4
1	A	251	TYR	2.3
1	C	207	SER	2.3
1	B	365	ILE	2.3
1	A	419	GLU	2.3
1	B	15	THR	2.3
1	C	280	ASN	2.3
1	C	277	ALA	2.3
1	A	292	TRP	2.3
1	C	256	PHE	2.3
1	B	228	LEU	2.3
1	B	37	GLY	2.2
1	A	356	VAL	2.2
1	C	91	ARG	2.2
1	C	275	ALA	2.2
1	C	361	LYS	2.2
1	A	417	GLU	2.2
1	A	343	PRO	2.2
1	B	82	LYS	2.2
1	B	356	VAL	2.2
1	A	345	ARG	2.2
1	A	415	ARG	2.1
1	B	36	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	348	ILE	2.1
1	A	342	LYS	2.1
1	C	419	GLU	2.1
1	B	149	PHE	2.1
1	C	404	LYS	2.1
1	C	231	VAL	2.1
1	C	220	ILE	2.1
1	B	415	ARG	2.1
1	C	225	GLU	2.1
1	B	330	GLN	2.1
1	C	384	GLN	2.1
1	B	133	PRO	2.1
1	C	217	PHE	2.1
1	C	227	PHE	2.1
1	B	63	ASP	2.1
1	B	273	GLY	2.1
1	C	274	VAL	2.0
1	C	381	ASP	2.0
1	C	347	SER	2.0
1	B	333	MET	2.0
1	C	292	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NA	A	421	1/1	0.94	0.24	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NA	C	421	1/1	0.95	0.18	-	8,8,8,8	0
2	NA	B	421	1/1	0.97	0.18	-	1,1,1,1	0

6.5 Other polymers (i)

There are no such residues in this entry.