Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 03:40 AM EDT

PDB ID	:	3R3I
Title	:	Crystal Structure of C-terminal truncation of UDP-glucose Pyrophosphorylase of Homo sapiens
Authors	:	Zheng, X.; Yu, Q.
Deposited on	:	2011-03-15
Resolution	:	3.57 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:

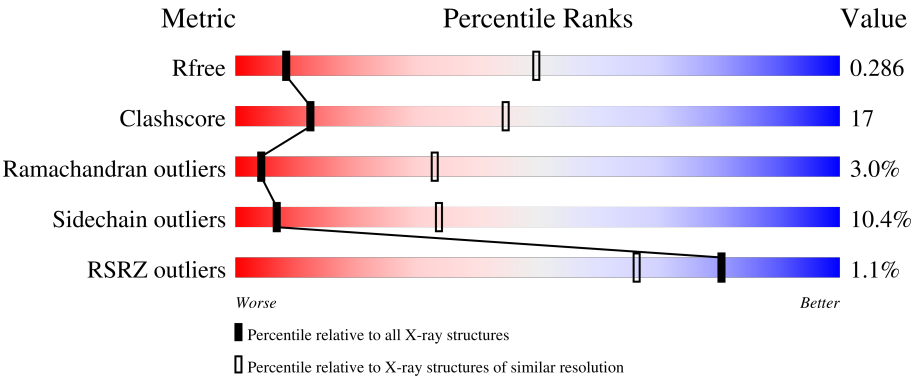
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.57 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}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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 <=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	528	55% 27% • 13%
1	B	528	52% 30% 5% 12%
1	C	528	3% 65% 16% • 17%
1	D	528	54% 27% 5% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13580 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3435	2190	577	658	10			
1	B	463	Total	C	N	O	S	0	0	0
			3468	2208	587	662	11			
1	C	439	Total	C	N	O	S	0	0	0
			3191	2027	528	627	9			
1	D	460	Total	C	N	O	S	0	0	0
			3486	2225	589	661	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	expression tag	UNP Q16851
A	-29	GLY	-	expression tag	UNP Q16851
A	-28	SER	-	expression tag	UNP Q16851
A	-27	SER	-	expression tag	UNP Q16851
A	-26	HIS	-	expression tag	UNP Q16851
A	-25	HIS	-	expression tag	UNP Q16851
A	-24	HIS	-	expression tag	UNP Q16851
A	-23	HIS	-	expression tag	UNP Q16851
A	-22	HIS	-	expression tag	UNP Q16851
A	-21	HIS	-	expression tag	UNP Q16851
A	-20	SER	-	expression tag	UNP Q16851
A	-19	SER	-	expression tag	UNP Q16851
A	-18	GLY	-	expression tag	UNP Q16851
A	-17	LEU	-	expression tag	UNP Q16851
A	-16	VAL	-	expression tag	UNP Q16851
A	-15	PRO	-	expression tag	UNP Q16851
A	-14	ARG	-	expression tag	UNP Q16851
A	-13	GLY	-	expression tag	UNP Q16851
A	-12	SER	-	expression tag	UNP Q16851
A	-11	HIS	-	expression tag	UNP Q16851
B	-30	MET	-	expression tag	UNP Q16851

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	GLY	-	expression tag	UNP Q16851
B	-28	SER	-	expression tag	UNP Q16851
B	-27	SER	-	expression tag	UNP Q16851
B	-26	HIS	-	expression tag	UNP Q16851
B	-25	HIS	-	expression tag	UNP Q16851
B	-24	HIS	-	expression tag	UNP Q16851
B	-23	HIS	-	expression tag	UNP Q16851
B	-22	HIS	-	expression tag	UNP Q16851
B	-21	HIS	-	expression tag	UNP Q16851
B	-20	SER	-	expression tag	UNP Q16851
B	-19	SER	-	expression tag	UNP Q16851
B	-18	GLY	-	expression tag	UNP Q16851
B	-17	LEU	-	expression tag	UNP Q16851
B	-16	VAL	-	expression tag	UNP Q16851
B	-15	PRO	-	expression tag	UNP Q16851
B	-14	ARG	-	expression tag	UNP Q16851
B	-13	GLY	-	expression tag	UNP Q16851
B	-12	SER	-	expression tag	UNP Q16851
B	-11	HIS	-	expression tag	UNP Q16851
C	-30	MET	-	expression tag	UNP Q16851
C	-29	GLY	-	expression tag	UNP Q16851
C	-28	SER	-	expression tag	UNP Q16851
C	-27	SER	-	expression tag	UNP Q16851
C	-26	HIS	-	expression tag	UNP Q16851
C	-25	HIS	-	expression tag	UNP Q16851
C	-24	HIS	-	expression tag	UNP Q16851
C	-23	HIS	-	expression tag	UNP Q16851
C	-22	HIS	-	expression tag	UNP Q16851
C	-21	HIS	-	expression tag	UNP Q16851
C	-20	SER	-	expression tag	UNP Q16851
C	-19	SER	-	expression tag	UNP Q16851
C	-18	GLY	-	expression tag	UNP Q16851
C	-17	LEU	-	expression tag	UNP Q16851
C	-16	VAL	-	expression tag	UNP Q16851
C	-15	PRO	-	expression tag	UNP Q16851
C	-14	ARG	-	expression tag	UNP Q16851
C	-13	GLY	-	expression tag	UNP Q16851
C	-12	SER	-	expression tag	UNP Q16851
C	-11	HIS	-	expression tag	UNP Q16851
D	-30	MET	-	expression tag	UNP Q16851
D	-29	GLY	-	expression tag	UNP Q16851
D	-28	SER	-	expression tag	UNP Q16851

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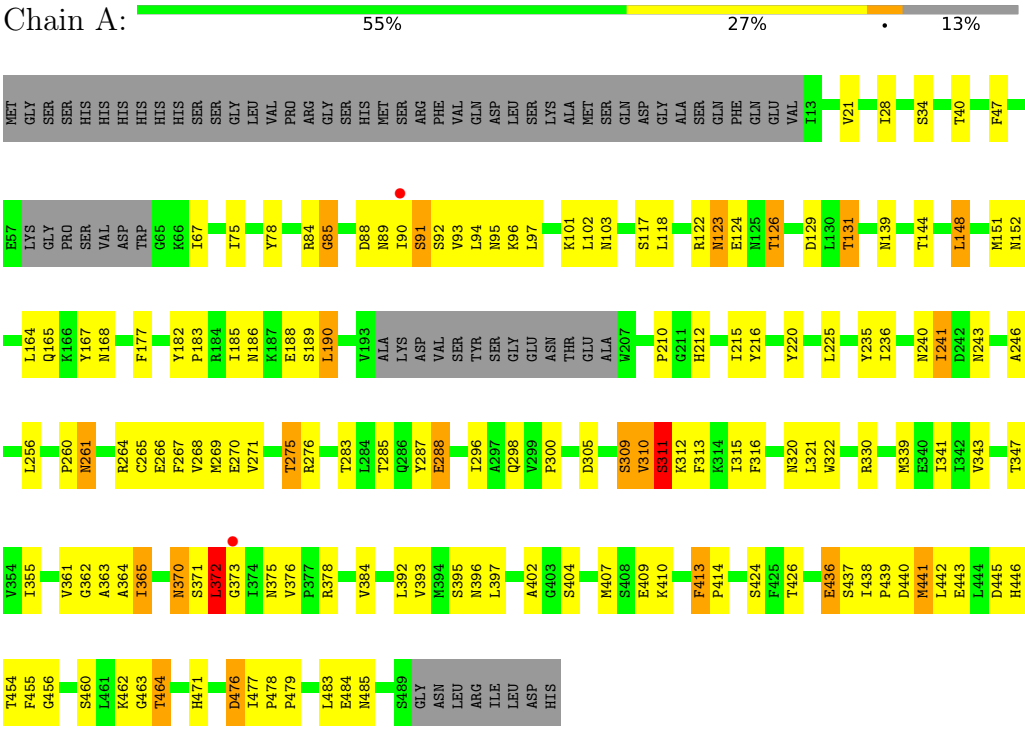
Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	SER	-	expression tag	UNP Q16851
D	-26	HIS	-	expression tag	UNP Q16851
D	-25	HIS	-	expression tag	UNP Q16851
D	-24	HIS	-	expression tag	UNP Q16851
D	-23	HIS	-	expression tag	UNP Q16851
D	-22	HIS	-	expression tag	UNP Q16851
D	-21	HIS	-	expression tag	UNP Q16851
D	-20	SER	-	expression tag	UNP Q16851
D	-19	SER	-	expression tag	UNP Q16851
D	-18	GLY	-	expression tag	UNP Q16851
D	-17	LEU	-	expression tag	UNP Q16851
D	-16	VAL	-	expression tag	UNP Q16851
D	-15	PRO	-	expression tag	UNP Q16851
D	-14	ARG	-	expression tag	UNP Q16851
D	-13	GLY	-	expression tag	UNP Q16851
D	-12	SER	-	expression tag	UNP Q16851
D	-11	HIS	-	expression tag	UNP Q16851

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.

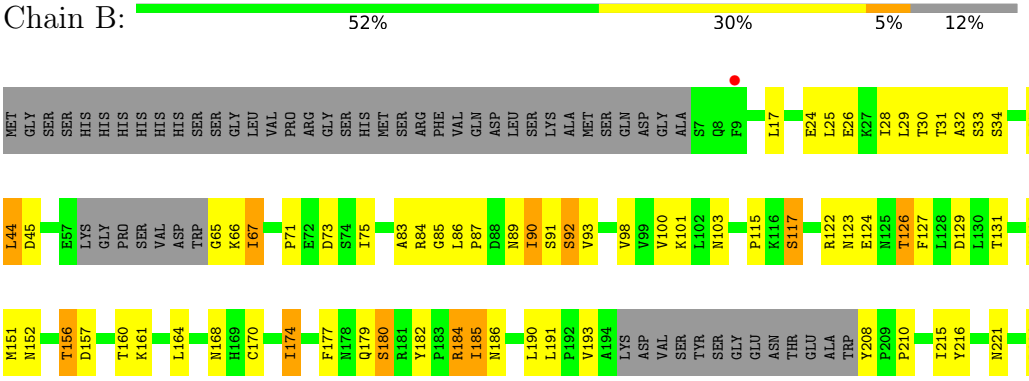
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

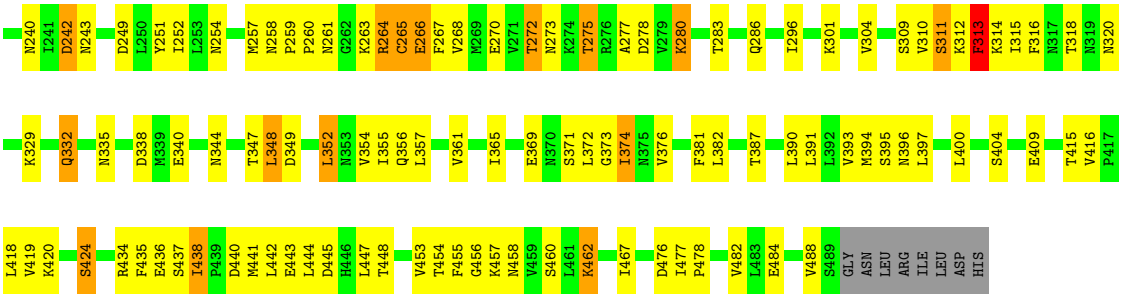
Chain A:



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

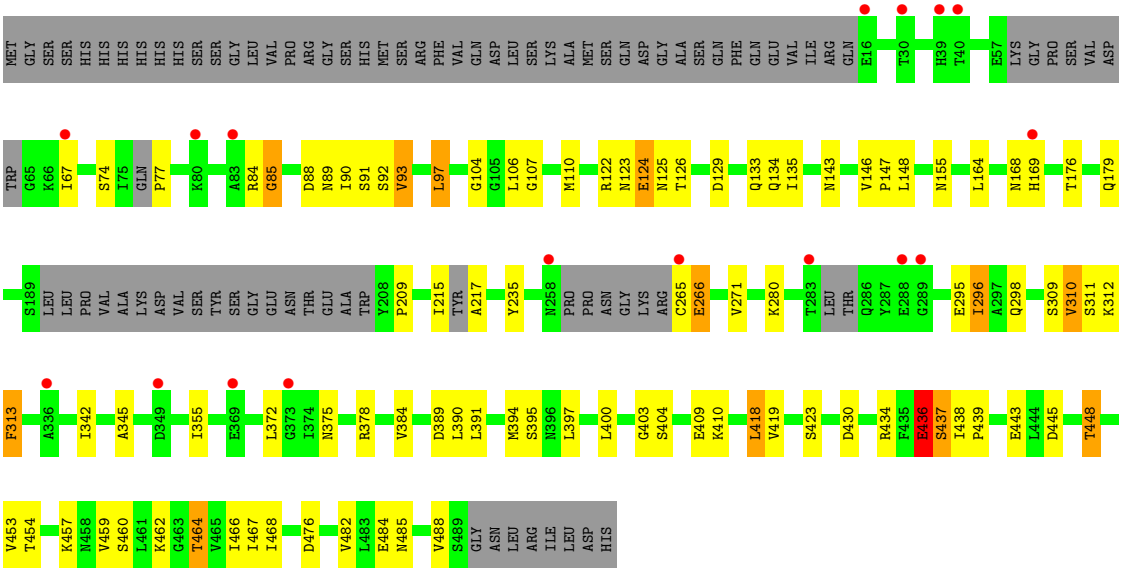
Chain B:





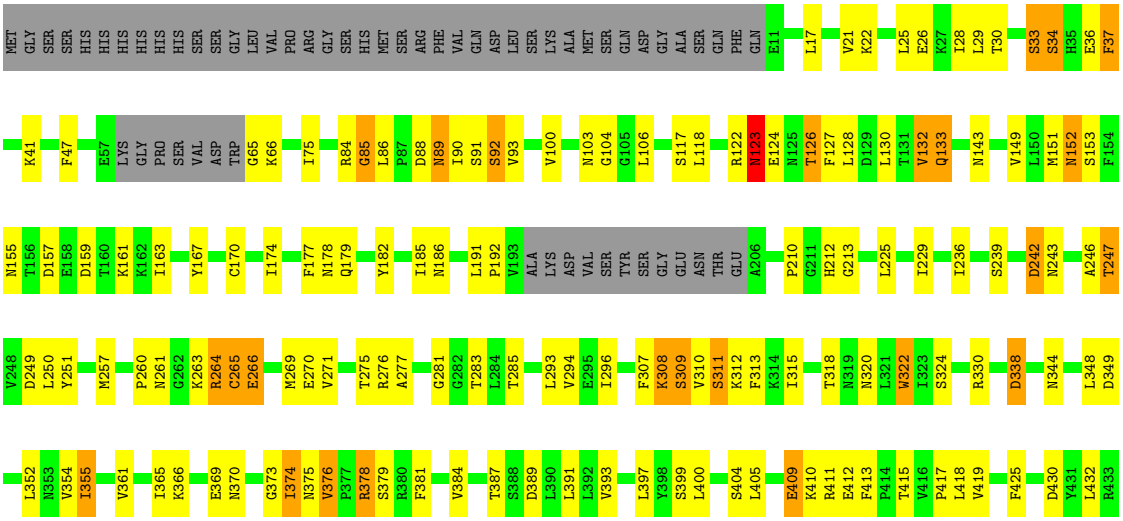
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain C:



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain D:




R434
F435
E436
S437
I438
M441
L442
E443
L444
D445
H446
L447
T448
T454
F455
G456
K457
N458
V459
S460
L461
K462
I466
N470
H471
D476
I477
V482
L483
E484
N485
K486
S489
GLY
ASN
LEU
ARG
ILE
LEU
ASP
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.27Å 140.27Å 315.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.57 19.98 – 3.57	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.98-3.57) 98.7 (19.98-3.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.233 , 0.286 0.229 , 0.286	Depositor DCC
R_{free} test set	2162 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	122.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 98.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13580	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.56	0/3496	0.71	3/4759 (0.1%)
1	B	0.64	1/3530 (0.0%)	0.81	1/4812 (0.0%)
1	C	0.47	0/3242	0.61	0/4429
1	D	0.69	0/3549	0.86	2/4831 (0.0%)
All	All	0.60	1/13817 (0.0%)	0.76	6/18831 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	424	SER	CB-OG	7.02	1.51	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	123	ASN	N-CA-C	5.45	125.70	111.00
1	D	405	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	372	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	123	ASN	N-CA-C	5.19	125.02	111.00
1	B	348	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	89	ASN	Peptide

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	3435	0	3332	114	0
1	B	3468	0	3341	143	0
1	C	3191	0	2963	70	0
1	D	3486	0	3410	127	1
All	All	13580	0	13046	450	1

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 17.

All (450) 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:265:CYS:CA	1:C:266:GLU:HB2	1.74	1.16
1:B:310:VAL:HB	1:B:312:LYS:HG3	1.26	1.12
1:C:265:CYS:HA	1:C:266:GLU:CB	1.80	1.11
1:A:413:PHE:CD2	1:A:414:PRO:HD2	1.91	1.04
1:A:264:ARG:NH1	1:A:372:LEU:HG	1.75	1.00
1:B:283:THR:HG22	1:B:315:ILE:O	1.61	1.00
1:B:84:ARG:H	1:B:85:GLY:HA2	1.29	0.98
1:B:438:ILE:HD12	1:B:438:ILE:H	1.25	0.96
1:C:91:SER:H	1:C:92:SER:HA	1.29	0.96
1:B:265:CYS:HA	1:B:266:GLU:HB2	1.49	0.95
1:A:264:ARG:NH2	1:A:371:SER:HA	1.82	0.94
1:A:264:ARG:HH11	1:A:372:LEU:HG	1.33	0.93
1:B:25:LEU:HB3	1:B:44:LEU:HD21	1.48	0.93
1:A:92:SER:N	1:A:93:VAL:HA	1.83	0.92
1:D:225:LEU:O	1:D:229:ILE:HG22	1.68	0.92
1:A:90:ILE:HA	1:A:91:SER:HB3	1.52	0.91
1:C:265:CYS:HA	1:C:266:GLU:HB2	0.94	0.91
1:D:310:VAL:HG12	1:D:312:LYS:HB2	1.56	0.86
1:A:309:SER:HA	1:A:310:VAL:C	1.96	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HH21	1:A:371:SER:HA	1.41	0.85
1:B:90:ILE:H	1:B:92:SER:HB2	1.42	0.85
1:D:275:THR:HG22	1:D:277:ALA:H	1.42	0.84
1:B:31:THR:H	1:B:32:ALA:HB3	1.41	0.84
1:A:161:LYS:HA	1:A:164:LEU:HD12	1.57	0.84
1:D:266:GLU:OE2	1:D:330:ARG:NH2	2.11	0.84
1:D:309:SER:HA	1:D:310:VAL:C	1.98	0.83
1:D:123:ASN:N	1:D:124:GLU:HA	1.92	0.83
1:B:265:CYS:HA	1:B:266:GLU:CB	2.08	0.83
1:B:252:ILE:HD13	1:B:374:ILE:HG12	1.61	0.83
1:B:348:LEU:HD12	1:B:349:ASP:HB3	1.58	0.83
1:D:90:ILE:H	1:D:91:SER:HA	1.41	0.82
1:B:156:THR:O	1:B:160:THR:HG23	1.80	0.81
1:D:90:ILE:N	1:D:91:SER:HA	1.93	0.81
1:D:186:ASN:HA	1:D:354:VAL:HG22	1.61	0.81
1:C:436:GLU:HA	1:C:436:GLU:OE1	1.80	0.80
1:D:265:CYS:HA	1:D:266:GLU:HB2	1.62	0.80
1:D:338:ASP:HB3	1:D:366:LYS:HE2	1.62	0.79
1:A:103:ASN:OD1	1:A:117:SER:OG	2.02	0.78
1:D:310:VAL:HG12	1:D:312:LYS:CB	2.12	0.78
1:D:430:ASP:O	1:D:434:ARG:HG2	1.84	0.78
1:D:457:LYS:HG3	1:D:458:ASN:ND2	1.99	0.78
1:B:123:ASN:N	1:B:124:GLU:HA	1.99	0.78
1:B:31:THR:N	1:B:32:ALA:HB3	2.00	0.77
1:B:309:SER:HB2	1:B:310:VAL:HA	1.65	0.76
1:A:454:THR:CG2	1:A:476:ASP:HB3	2.15	0.76
1:B:122:ARG:HH21	1:B:394:MET:HA	1.49	0.76
1:A:477:ILE:HD11	1:A:483:LEU:HD21	1.67	0.76
1:B:462:LYS:O	1:B:484:GLU:HA	1.86	0.75
1:B:438:ILE:HD12	1:B:438:ILE:N	1.99	0.75
1:D:318:THR:HG23	1:D:381:PHE:CD1	2.21	0.75
1:A:409:GLU:HB3	1:A:410:LYS:HA	1.67	0.74
1:A:92:SER:H	1:A:93:VAL:HA	1.51	0.74
1:A:123:ASN:N	1:A:124:GLU:HA	2.00	0.74
1:B:252:ILE:CD1	1:B:374:ILE:HG12	2.17	0.74
1:D:263:LYS:HA	1:D:264:ARG:CB	2.17	0.74
1:D:443:GLU:HB2	1:D:462:LYS:HG2	1.70	0.74
1:D:84:ARG:H	1:D:85:GLY:HA2	1.53	0.73
1:C:462:LYS:HB2	1:C:484:GLU:HG3	1.70	0.73
1:C:390:LEU:O	1:C:394:MET:HG2	1.89	0.73
1:A:90:ILE:HA	1:A:91:SER:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:THR:HG23	1:D:381:PHE:HD1	1.54	0.72
1:A:413:PHE:HD2	1:A:414:PRO:HD2	1.51	0.72
1:B:90:ILE:N	1:B:91:SER:HA	2.02	0.72
1:D:454:THR:HG22	1:D:476:ASP:HA	1.69	0.72
1:A:103:ASN:HD21	1:A:160:THR:HG21	1.55	0.72
1:B:266:GLU:HG2	1:B:369:GLU:O	1.90	0.72
1:B:25:LEU:HD22	1:B:44:LEU:HD11	1.71	0.71
1:B:267:PHE:CE2	1:B:365:ILE:HG12	2.24	0.71
1:C:91:SER:N	1:C:92:SER:HA	1.96	0.71
1:A:454:THR:HG23	1:A:476:ASP:HB3	1.70	0.71
1:B:240:ASN:HB3	1:B:242:ASP:OD2	1.90	0.71
1:C:122:ARG:HD2	1:C:400:LEU:HD13	1.73	0.70
1:B:348:LEU:HD12	1:B:349:ASP:CB	2.21	0.70
1:D:265:CYS:HA	1:D:266:GLU:CB	2.21	0.70
1:B:313:PHE:H	1:B:313:PHE:HD2	1.39	0.69
1:D:312:LYS:HD3	1:D:313:PHE:HE2	1.58	0.69
1:C:92:SER:HB2	1:C:93:VAL:HB	1.73	0.68
1:A:276:ARG:NH2	1:C:443:GLU:HB3	2.08	0.68
1:A:271:VAL:HG11	1:A:315:ILE:HG23	1.76	0.67
1:D:90:ILE:N	1:D:91:SER:CA	2.57	0.67
1:D:151:MET:HG3	1:D:177:PHE:CE1	2.29	0.67
1:A:446:HIS:HB3	1:A:464:THR:HG22	1.76	0.67
1:D:84:ARG:H	1:D:85:GLY:CA	2.07	0.67
1:B:332:GLN:HA	1:B:332:GLN:NE2	2.10	0.66
1:A:102:LEU:O	1:A:241:ILE:HG13	1.96	0.66
1:D:448:THR:CG2	1:D:466:ILE:HG12	2.24	0.66
1:B:28:ILE:HA	1:B:31:THR:OG1	1.95	0.66
1:B:103:ASN:HB3	1:B:152:ASN:HB3	1.77	0.66
1:C:418:LEU:HD23	1:C:419:VAL:H	1.60	0.66
1:B:24:GLU:OE1	1:B:191:LEU:HG	1.97	0.65
1:D:283:THR:HG21	1:D:313:PHE:HD1	1.62	0.65
1:D:22:LYS:O	1:D:26:GLU:HG2	1.96	0.65
1:A:156:THR:O	1:A:160:THR:HG23	1.96	0.65
1:D:310:VAL:CG1	1:D:312:LYS:HB2	2.27	0.65
1:A:75:ILE:HA	1:A:373:GLY:O	1.97	0.64
1:D:242:ASP:N	1:D:242:ASP:OD1	2.29	0.64
1:D:312:LYS:HD3	1:D:313:PHE:CE2	2.32	0.64
1:A:447:LEU:HD11	1:A:449:VAL:HG12	1.80	0.64
1:C:434:ARG:HD2	1:C:453:VAL:O	1.98	0.64
1:D:122:ARG:O	1:D:123:ASN:HB2	1.98	0.63
1:D:270:GLU:OE1	1:D:322:TRP:HZ3	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:O	1:A:361:VAL:HG23	1.99	0.62
1:D:126:THR:HG23	1:D:128:LEU:H	1.64	0.62
1:D:266:GLU:OE1	1:D:369:GLU:HB3	2.00	0.62
1:B:151:MET:HG3	1:B:177:PHE:CZ	2.35	0.62
1:A:122:ARG:C	1:A:124:GLU:HA	2.21	0.61
1:A:264:ARG:NH2	1:A:371:SER:CA	2.61	0.61
1:A:264:ARG:HB3	1:A:265:CYS:HA	1.82	0.61
1:D:191:LEU:HG	1:D:192:PRO:HD2	1.81	0.61
1:D:378:ARG:O	1:D:378:ARG:HG3	1.99	0.61
1:D:391:LEU:HD23	1:D:419:VAL:HG11	1.83	0.61
1:B:174:ILE:HD13	1:B:174:ILE:H	1.66	0.61
1:A:395:SER:OG	1:A:441:MET:HG3	2.01	0.60
1:D:130:LEU:O	1:D:133:GLN:HB2	2.01	0.60
1:A:448:THR:HG21	1:C:466:ILE:CD1	2.32	0.60
1:C:179:GLN:HE22	1:C:209:PRO:HB3	1.67	0.60
1:C:179:GLN:NE2	1:C:209:PRO:HB3	2.17	0.60
1:A:384:VAL:HG12	1:A:384:VAL:O	2.02	0.60
1:A:92:SER:N	1:A:93:VAL:CA	2.62	0.59
1:B:174:ILE:HD13	1:B:174:ILE:N	2.17	0.59
1:A:264:ARG:NH2	1:A:372:LEU:H	2.00	0.59
1:A:264:ARG:HB3	1:A:265:CYS:SG	2.42	0.59
1:B:31:THR:CA	1:B:32:ALA:HB3	2.31	0.59
1:B:103:ASN:OD1	1:B:117:SER:OG	2.20	0.59
1:B:435:PHE:HB3	1:B:437:SER:O	2.02	0.59
1:C:92:SER:H	1:C:93:VAL:HB	1.67	0.59
1:B:268:VAL:HA	1:B:372:LEU:O	2.02	0.59
1:A:256:LEU:HD21	1:A:268:VAL:HG21	1.84	0.59
1:B:443:GLU:HB2	1:B:462:LYS:HB3	1.83	0.59
1:D:88:ASP:CG	1:D:89:ASN:H	2.07	0.58
1:B:260:PRO:O	1:B:261:ASN:HB2	2.02	0.58
1:A:101:LYS:HD2	1:A:131:THR:HG21	1.85	0.58
1:B:263:LYS:HA	1:B:264:ARG:CB	2.33	0.58
1:A:264:ARG:HG2	1:A:370:ASN:ND2	2.19	0.58
1:C:97:LEU:HD12	1:C:235:TYR:HB2	1.84	0.58
1:A:151:MET:HG3	1:A:177:PHE:CE1	2.38	0.58
1:B:84:ARG:N	1:B:85:GLY:HA2	2.03	0.58
1:B:454:THR:HG22	1:B:476:ASP:OD2	2.03	0.58
1:D:25:LEU:HA	1:D:28:ILE:HD12	1.84	0.58
1:A:264:ARG:HB3	1:A:265:CYS:CA	2.34	0.58
1:D:271:VAL:O	1:D:375:ASN:HA	2.04	0.58
1:D:153:SER:HB3	1:D:179:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:THR:H	1:A:129:ASP:HB2	1.69	0.57
1:B:161:LYS:HA	1:B:164:LEU:HD12	1.85	0.57
1:B:243:ASN:HD21	1:B:381:PHE:HA	1.69	0.57
1:B:151:MET:HG3	1:B:177:PHE:CE1	2.40	0.57
1:B:184:ARG:H	1:B:184:ARG:HD2	1.70	0.57
1:B:313:PHE:N	1:B:313:PHE:CD2	2.73	0.57
1:D:33:SER:O	1:D:34:SER:C	2.42	0.57
1:B:272:THR:HG22	1:B:273:ASN:H	1.69	0.57
1:A:264:ARG:NH2	1:A:372:LEU:N	2.53	0.57
1:A:92:SER:H	1:A:93:VAL:CA	2.18	0.56
1:B:86:LEU:HB3	1:B:251:TYR:CE1	2.40	0.56
1:D:75:ILE:HA	1:D:373:GLY:O	2.05	0.56
1:B:91:SER:HA	1:B:92:SER:HB2	1.87	0.56
1:B:84:ARG:H	1:B:85:GLY:CA	2.10	0.56
1:D:281:GLY:O	1:D:307:PHE:HZ	1.88	0.56
1:C:133:GLN:HB3	1:C:403:GLY:HA3	1.87	0.56
1:C:90:ILE:HD11	1:C:143:ASN:HD22	1.70	0.56
1:B:122:ARG:C	1:B:124:GLU:HA	2.25	0.55
1:B:122:ARG:HD2	1:B:400:LEU:HB2	1.88	0.55
1:B:270:GLU:HB2	1:B:320:ASN:HB2	1.88	0.55
1:A:188:GLU:H	1:A:352:LEU:HD21	1.71	0.55
1:B:91:SER:HA	1:B:92:SER:CB	2.36	0.55
1:D:283:THR:HG23	1:D:315:ILE:HB	1.89	0.55
1:D:374:ILE:HG13	1:D:374:ILE:O	2.07	0.55
1:B:26:GLU:HA	1:B:29:LEU:HD12	1.88	0.54
1:D:103:ASN:HB3	1:D:152:ASN:HB3	1.89	0.54
1:A:448:THR:HG21	1:C:466:ILE:HD11	1.89	0.54
1:D:89:ASN:O	1:D:91:SER:HB3	2.08	0.54
1:C:135:ILE:HG13	1:C:148:LEU:HD11	1.89	0.54
1:B:208:TYR:CE1	1:B:356:GLN:HG3	2.43	0.54
1:B:355:ILE:HG22	1:B:356:GLN:N	2.23	0.54
1:B:438:ILE:H	1:B:438:ILE:CD1	2.05	0.54
1:D:384:VAL:HG12	1:D:384:VAL:O	2.08	0.54
1:A:455:PHE:HA	1:A:477:ILE:HG22	1.89	0.53
1:B:90:ILE:N	1:B:92:SER:HB2	2.17	0.53
1:B:185:ILE:HG13	1:B:186:ASN:N	2.22	0.53
1:C:436:GLU:O	1:C:437:SER:CB	2.57	0.53
1:D:117:SER:O	1:D:127:PHE:HB2	2.08	0.53
1:C:295:GLU:HB2	1:C:298:GLN:HE21	1.73	0.53
1:C:468:ILE:HG22	1:C:468:ILE:O	2.09	0.53
1:B:182:TYR:HE2	1:B:210:PRO:HG3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG13	1:B:257:MET:HG2	1.90	0.53
1:D:29:LEU:HD11	1:D:41:LYS:HG3	1.89	0.53
1:B:184:ARG:O	1:B:193:VAL:HG23	2.09	0.53
1:B:457:LYS:O	1:B:458:ASN:HB2	2.09	0.53
1:D:249:ASP:OD1	1:D:250:LEU:N	2.41	0.53
1:D:271:VAL:O	1:D:376:VAL:HG23	2.08	0.53
1:A:438:ILE:HD12	1:A:438:ILE:H	1.74	0.53
1:A:362:GLY:O	1:A:365:ILE:HG13	2.09	0.52
1:A:185:ILE:HG13	1:A:186:ASN:N	2.24	0.52
1:B:71:PRO:HD3	1:B:286:GLN:HB2	1.91	0.52
1:B:332:GLN:HA	1:B:332:GLN:HE21	1.73	0.52
1:D:90:ILE:HB	1:D:92:SER:HB2	1.91	0.52
1:D:276:ARG:HH11	1:D:276:ARG:HG3	1.74	0.52
1:B:32:ALA:C	1:B:34:SER:H	2.12	0.52
1:A:185:ILE:HG13	1:A:186:ASN:H	1.74	0.52
1:B:273:ASN:HA	1:B:314:LYS:O	2.09	0.52
1:D:90:ILE:HB	1:D:92:SER:CB	2.40	0.52
1:D:310:VAL:HG12	1:D:312:LYS:HB3	1.92	0.52
1:B:265:CYS:CA	1:B:266:GLU:CB	2.84	0.52
1:A:264:ARG:CZ	1:A:372:LEU:N	2.73	0.52
1:C:92:SER:N	1:C:93:VAL:HB	2.24	0.51
1:D:249:ASP:OD1	1:D:249:ASP:C	2.48	0.51
1:D:151:MET:HG3	1:D:177:PHE:CZ	2.46	0.51
1:D:229:ILE:HG13	1:D:229:ILE:O	2.10	0.51
1:D:265:CYS:O	1:D:265:CYS:SG	2.69	0.51
1:B:89:ASN:O	1:B:93:VAL:HG23	2.11	0.51
1:C:311:SER:HA	1:C:313:PHE:N	2.26	0.51
1:D:265:CYS:CA	1:D:266:GLU:CB	2.89	0.51
1:A:362:GLY:O	1:A:364:ALA:N	2.43	0.51
1:A:362:GLY:C	1:A:364:ALA:H	2.13	0.51
1:C:92:SER:CB	1:C:93:VAL:HB	2.39	0.51
1:A:126:THR:HG22	1:A:129:ASP:H	1.75	0.51
1:A:462:LYS:O	1:A:484:GLU:HA	2.11	0.50
1:B:249:ASP:OD2	1:B:252:ILE:HG22	2.10	0.50
1:B:75:ILE:HA	1:B:373:GLY:O	2.11	0.50
1:A:84:ARG:H	1:A:85:GLY:CA	2.25	0.50
1:B:115:PRO:HB3	1:B:156:THR:HG22	1.94	0.50
1:D:182:TYR:CD2	1:D:210:PRO:HG3	2.46	0.50
1:D:344:ASN:O	1:D:355:ILE:HA	2.11	0.50
1:A:220:TYR:HD1	1:A:225:LEU:HD23	1.75	0.50
1:A:276:ARG:HH22	1:C:443:GLU:HB3	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ARG:N	1:D:85:GLY:CA	2.71	0.50
1:A:139:ASN:OD1	1:A:144:THR:HG23	2.12	0.50
1:C:92:SER:CA	1:C:93:VAL:HB	2.41	0.50
1:A:264:ARG:NH2	1:A:267:PHE:O	2.45	0.49
1:B:31:THR:HB	1:B:32:ALA:HB3	1.93	0.49
1:B:226:ASP:HA	1:B:229:ILE:HG22	1.93	0.49
1:B:270:GLU:HB3	1:B:376:VAL:HG21	1.93	0.49
1:B:436:GLU:OE1	1:B:456:GLY:HA2	2.11	0.49
1:D:47:PHE:HD1	1:D:182:TYR:HD1	1.58	0.49
1:C:464:THR:O	1:C:485:ASN:HA	2.12	0.49
1:A:267:PHE:CD2	1:A:365:ILE:HG23	2.47	0.49
1:B:90:ILE:HD12	1:B:92:SER:HB3	1.95	0.49
1:B:460:SER:HB3	1:B:482:VAL:HG22	1.95	0.49
1:C:418:LEU:CD2	1:C:419:VAL:H	2.25	0.49
1:D:447:LEU:HD22	1:D:461:LEU:HD13	1.95	0.49
1:A:352:LEU:HD23	1:A:353:ASN:N	2.28	0.49
1:B:43:ASP:OD1	1:B:180:SER:HB3	2.13	0.49
1:B:312:LYS:O	1:B:314:LYS:N	2.46	0.49
1:D:118:LEU:C	1:D:126:THR:OG1	2.51	0.49
1:B:182:TYR:CE2	1:B:210:PRO:HG3	2.49	0.48
1:D:89:ASN:HA	1:D:90:ILE:HA	1.44	0.48
1:B:249:ASP:HB3	1:B:252:ILE:HG22	1.95	0.48
1:D:122:ARG:C	1:D:124:GLU:HA	2.33	0.48
1:D:309:SER:CA	1:D:310:VAL:C	2.77	0.48
1:B:208:TYR:CD1	1:B:356:GLN:HG3	2.49	0.48
1:B:215:ILE:HG23	1:B:216:TYR:N	2.29	0.48
1:B:83:ALA:O	1:B:84:ARG:HG3	2.14	0.48
1:A:309:SER:HA	1:A:310:VAL:O	2.13	0.48
1:C:123:ASN:HA	1:C:124:GLU:HA	1.53	0.48
1:D:309:SER:HA	1:D:311:SER:N	2.28	0.48
1:D:283:THR:HG21	1:D:313:PHE:CD1	2.46	0.47
1:B:84:ARG:N	1:B:85:GLY:CA	2.75	0.47
1:D:153:SER:O	1:D:155:ASN:N	2.48	0.47
1:A:396:ASN:OD1	1:A:440:ASP:HA	2.15	0.47
1:B:453:VAL:HG12	1:B:454:THR:N	2.29	0.47
1:D:435:PHE:CE1	1:D:455:PHE:CD2	3.02	0.47
1:A:129:ASP:OD1	1:A:167:TYR:OH	2.21	0.47
1:B:355:ILE:CG2	1:B:356:GLN:N	2.78	0.47
1:A:243:ASN:HD22	1:A:320:ASN:HD21	1.63	0.47
1:B:467:ILE:HG23	1:B:488:VAL:HB	1.96	0.47
1:B:90:ILE:N	1:B:91:SER:CA	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HG3	1:B:208:TYR:CD2	2.50	0.47
1:D:271:VAL:HG11	1:D:315:ILE:HG23	1.96	0.47
1:A:78:TYR:HB2	1:A:375:ASN:O	2.15	0.47
1:A:84:ARG:N	1:A:85:GLY:CA	2.78	0.47
1:B:454:THR:CG2	1:B:476:ASP:OD2	2.63	0.47
1:D:47:PHE:HA	1:D:182:TYR:HE1	1.79	0.47
1:B:174:ILE:H	1:B:174:ILE:CD1	2.26	0.47
1:C:215:ILE:O	1:C:217:ALA:N	2.49	0.46
1:C:77:PRO:HA	1:C:375:ASN:HB3	1.96	0.46
1:C:168:ASN:O	1:C:169:HIS:HB2	2.16	0.46
1:C:311:SER:HA	1:C:313:PHE:H	1.79	0.46
1:D:270:GLU:HB2	1:D:320:ASN:HB2	1.96	0.46
1:D:91:SER:C	1:D:93:VAL:H	2.17	0.46
1:D:152:ASN:O	1:D:178:ASN:HA	2.15	0.46
1:D:265:CYS:HB3	1:D:370:ASN:HD22	1.80	0.46
1:D:443:GLU:CB	1:D:462:LYS:HG2	2.43	0.46
1:A:185:ILE:HG23	1:A:355:ILE:HB	1.97	0.46
1:B:98:VAL:HB	1:B:236:ILE:HG12	1.97	0.46
1:B:332:GLN:NE2	1:B:332:GLN:CA	2.78	0.46
1:C:394:MET:HG3	1:C:438:ILE:HG13	1.96	0.46
1:A:447:LEU:HD12	1:A:448:THR:N	2.31	0.46
1:D:413:PHE:CD2	1:D:413:PHE:N	2.83	0.46
1:D:462:LYS:HB2	1:D:484:GLU:HG3	1.98	0.46
1:A:447:LEU:HD11	1:A:449:VAL:CG1	2.46	0.46
1:B:31:THR:HB	1:B:32:ALA:CB	2.44	0.46
1:A:264:ARG:CB	1:A:265:CYS:HA	2.41	0.46
1:B:419:VAL:HG22	1:B:447:LEU:HB3	1.98	0.46
1:D:122:ARG:HD2	1:D:400:LEU:HD22	1.98	0.46
1:D:270:GLU:OE1	1:D:322:TRP:CZ3	2.65	0.46
1:D:271:VAL:CG1	1:D:315:ILE:HG23	2.46	0.46
1:A:249:ASP:HB3	1:A:252:ILE:HD12	1.98	0.45
1:B:355:ILE:CG2	1:B:356:GLN:H	2.28	0.45
1:B:391:LEU:HG	1:B:441:MET:HE2	1.97	0.45
1:D:409:GLU:HA	1:D:410:LYS:HA	1.56	0.45
1:D:348:LEU:HB3	1:D:349:ASP:OD1	2.16	0.45
1:D:397:LEU:HD11	1:D:417:PRO:HG3	1.98	0.45
1:B:311:SER:H	1:B:312:LYS:HB2	1.81	0.45
1:D:157:ASP:OD2	1:D:161:LYS:HD2	2.17	0.45
1:D:167:TYR:O	1:D:170:CYS:HB2	2.16	0.45
1:B:126:THR:O	1:B:129:ASP:N	2.49	0.45
1:B:90:ILE:H	1:B:90:ILE:HG13	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:O	1:C:125:ASN:N	2.48	0.45
1:D:271:VAL:H	1:D:376:VAL:CG2	2.29	0.45
1:B:301:LYS:O	1:B:304:VAL:HG23	2.16	0.45
1:A:215:ILE:HG23	1:A:216:TYR:N	2.32	0.45
1:D:448:THR:HG23	1:D:466:ILE:HG12	1.97	0.45
1:D:36:GLU:O	1:D:37:PHE:HB2	2.17	0.45
1:D:65:GLY:HA3	1:D:66:LYS:HA	1.73	0.45
1:D:378:ARG:O	1:D:378:ARG:CG	2.65	0.45
1:C:126:THR:HG22	1:C:129:ASP:OD2	2.17	0.44
1:A:182:TYR:CD2	1:A:210:PRO:HB3	2.52	0.44
1:C:391:LEU:HD12	1:C:438:ILE:HD12	2.00	0.44
1:C:409:GLU:HA	1:C:410:LYS:HA	1.64	0.44
1:A:53:ARG:HB3	1:A:341:ILE:HD11	1.99	0.44
1:A:365:ILE:HG22	1:A:371:SER:OG	2.16	0.44
1:C:84:ARG:N	1:C:85:GLY:CA	2.79	0.44
1:D:17:LEU:O	1:D:21:VAL:HG23	2.17	0.44
1:D:437:SER:HB3	1:D:457:LYS:HA	1.98	0.44
1:C:448:THR:HG23	1:C:466:ILE:HG12	1.99	0.44
1:D:212:HIS:ND1	1:D:361:VAL:HG23	2.32	0.44
1:A:298:GLN:O	1:A:300:PRO:HD3	2.17	0.44
1:C:107:GLY:O	1:C:110:MET:HB2	2.18	0.44
1:C:296:ILE:H	1:C:296:ILE:HG13	1.49	0.44
1:A:47:PHE:CD1	1:A:183:PRO:HD2	2.52	0.44
1:B:332:GLN:HE21	1:B:332:GLN:CA	2.30	0.44
1:C:106:LEU:HD21	1:C:155:ASN:OD1	2.17	0.44
1:A:260:PRO:O	1:A:261:ASN:C	2.56	0.44
1:B:101:LYS:HE3	1:B:131:THR:HG23	2.00	0.44
1:B:148:LEU:HD23	1:B:149:VAL:N	2.33	0.44
1:A:88:ASP:HA	1:A:89:ASN:HA	1.80	0.44
1:A:270:GLU:OE1	1:A:320:ASN:HB3	2.18	0.44
1:A:409:GLU:HB3	1:A:410:LYS:CA	2.43	0.44
1:C:91:SER:N	1:C:92:SER:CA	2.74	0.44
1:C:280:LYS:HB3	1:C:296:ILE:HD13	2.00	0.44
1:D:86:LEU:HD13	1:D:251:TYR:CZ	2.53	0.44
1:A:309:SER:CA	1:A:310:VAL:C	2.80	0.43
1:B:278:ASP:OD1	1:B:278:ASP:N	2.50	0.43
1:C:90:ILE:HA	1:C:91:SER:HA	1.55	0.43
1:D:348:LEU:HA	1:D:349:ASP:HA	1.65	0.43
1:B:396:ASN:ND2	1:B:440:ASP:OD1	2.44	0.43
1:C:454:THR:HG22	1:C:476:ASP:HA	2.00	0.43
1:C:454:THR:HG22	1:C:476:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:O	1:A:54:PHE:HB3	2.19	0.43
1:A:92:SER:H	1:A:93:VAL:C	2.21	0.43
1:B:310:VAL:CB	1:B:312:LYS:HG3	2.19	0.43
1:B:441:MET:O	1:B:442:LEU:HB2	2.18	0.43
1:C:122:ARG:HH11	1:C:400:LEU:HB2	1.83	0.43
1:A:103:ASN:ND2	1:A:160:THR:HG21	2.29	0.43
1:B:184:ARG:HG3	1:B:208:TYR:HD2	1.83	0.43
1:B:390:LEU:O	1:B:393:VAL:HG12	2.18	0.43
1:B:420:LYS:HE2	1:B:420:LYS:HB3	1.85	0.43
1:C:92:SER:H	1:C:93:VAL:CB	2.31	0.43
1:D:269:MET:SD	1:D:365:ILE:HD11	2.59	0.43
1:D:293:LEU:HG	1:D:294:VAL:N	2.33	0.43
1:D:444:LEU:HD22	1:D:445:ASP:N	2.33	0.43
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.77	0.43
1:C:460:SER:HB3	1:C:482:VAL:HG22	1.99	0.43
1:A:126:THR:N	1:A:129:ASP:HB2	2.31	0.43
1:B:65:GLY:HA3	1:B:66:LYS:HA	1.66	0.43
1:B:265:CYS:CA	1:B:266:GLU:HB2	2.34	0.43
1:B:266:GLU:OE1	1:B:369:GLU:HG2	2.18	0.43
1:B:395:SER:OG	1:B:441:MET:HG3	2.19	0.43
1:C:437:SER:OG	1:C:457:LYS:HA	2.19	0.43
1:B:267:PHE:CD2	1:B:365:ILE:HG12	2.54	0.43
1:A:347:THR:HB	1:A:353:ASN:OD1	2.19	0.43
1:C:88:ASP:HA	1:C:89:ASN:HA	1.74	0.43
1:A:311:SER:C	1:A:313:PHE:H	2.21	0.43
1:A:463:GLY:HA3	1:A:485:ASN:OD1	2.19	0.43
1:B:272:THR:HG22	1:B:273:ASN:N	2.33	0.43
1:D:311:SER:HA	1:D:313:PHE:N	2.34	0.43
1:B:435:PHE:CE1	1:B:455:PHE:CD2	3.07	0.43
1:A:436:GLU:HG3	1:A:456:GLY:HA2	1.99	0.42
1:C:146:VAL:HA	1:C:147:PRO:HD3	1.81	0.42
1:D:409:GLU:HA	1:D:411:ARG:H	1.84	0.42
1:D:470:ASN:O	1:D:471:HIS:C	2.57	0.42
1:A:287:TYR:O	1:A:288:GLU:HB2	2.18	0.42
1:A:477:ILE:CD1	1:A:483:LEU:HD11	2.48	0.42
1:B:477:ILE:HA	1:B:478:PRO:HD3	1.88	0.42
1:C:384:VAL:HG13	1:C:389:ASP:HB2	2.01	0.42
1:C:345:ALA:HB2	1:C:355:ILE:HG12	2.01	0.42
1:C:409:GLU:HA	1:C:409:GLU:OE1	2.19	0.42
1:A:252:ILE:HD13	1:A:322:TRP:CH2	2.55	0.42
1:A:441:MET:O	1:A:443:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LEU:O	1:D:132:VAL:HG13	2.20	0.42
1:D:387:THR:HG21	1:D:425:PHE:O	2.19	0.42
1:A:97:LEU:HA	1:A:235:TYR:O	2.20	0.42
1:A:339:MET:CG	1:A:364:ALA:HB2	2.50	0.42
1:A:409:GLU:HA	1:A:410:LYS:C	2.40	0.42
1:D:444:LEU:HD11	1:D:447:LEU:HB2	2.00	0.42
1:B:98:VAL:HG12	1:B:100:VAL:HG23	2.02	0.42
1:B:168:ASN:C	1:B:170:CYS:H	2.23	0.42
1:B:348:LEU:HA	1:B:349:ASP:HA	1.75	0.42
1:D:93:VAL:HG22	1:D:257:MET:HG3	2.01	0.42
1:D:276:ARG:HG3	1:D:276:ARG:NH1	2.34	0.42
1:C:419:VAL:O	1:C:419:VAL:HG23	2.19	0.42
1:A:91:SER:HA	1:A:92:SER:HA	1.62	0.42
1:B:157:ASP:OD1	1:B:157:ASP:C	2.58	0.41
1:B:280:LYS:O	1:B:296:ILE:HD11	2.19	0.41
1:C:467:ILE:HG23	1:C:488:VAL:HB	2.02	0.41
1:D:250:LEU:HA	1:D:250:LEU:HD23	1.87	0.41
1:B:409:GLU:H	1:B:409:GLU:HG3	1.40	0.41
1:D:384:VAL:HG22	1:D:389:ASP:HB3	2.02	0.41
1:A:438:ILE:HA	1:A:439:PRO:HD3	1.83	0.41
1:B:174:ILE:N	1:B:174:ILE:CD1	2.82	0.41
1:B:272:THR:HG23	1:B:376:VAL:O	2.20	0.41
1:C:134:GLN:HG2	1:C:404:SER:HB3	2.02	0.41
1:A:186:ASN:O	1:A:190:LEU:HA	2.20	0.41
1:A:269:MET:H	1:A:373:GLY:HA2	1.85	0.41
1:B:348:LEU:HD12	1:B:349:ASP:CA	2.50	0.41
1:D:260:PRO:O	1:D:261:ASN:CB	2.68	0.41
1:D:308:LYS:O	1:D:309:SER:HB3	2.20	0.41
1:A:275:THR:OG1	1:A:378:ARG:NH2	2.53	0.41
1:B:87:PRO:HD3	1:B:254:ASN:HB2	2.03	0.41
1:A:266:GLU:OE1	1:A:330:ARG:NH2	2.53	0.41
1:D:100:VAL:HG22	1:D:149:VAL:HB	2.02	0.41
1:D:271:VAL:H	1:D:376:VAL:HG23	1.84	0.41
1:A:271:VAL:HG22	1:A:316:PHE:O	2.20	0.41
1:D:425:PHE:N	1:D:425:PHE:CD2	2.89	0.41
1:A:478:PRO:HA	1:A:479:PRO:HD3	1.94	0.41
1:B:73:ASP:N	1:B:73:ASP:OD1	2.53	0.41
1:B:275:THR:HB	1:B:277:ALA:HB3	2.03	0.41
1:D:265:CYS:HB2	1:D:370:ASN:HB3	2.03	0.41
1:B:17:LEU:HD21	1:B:190:LEU:HD13	2.02	0.41
1:B:31:THR:CA	1:B:32:ALA:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASN:OD1	1:B:258:ASN:O	2.39	0.41
1:C:271:VAL:HG23	1:C:375:ASN:HA	2.03	0.41
1:C:438:ILE:HA	1:C:439:PRO:HD3	1.95	0.41
1:B:259:PRO:HA	1:B:260:PRO:HD3	1.76	0.41
1:C:309:SER:HA	1:C:310:VAL:HA	1.60	0.41
1:A:270:GLU:HB2	1:A:320:ASN:HB2	2.03	0.40
1:D:460:SER:HB3	1:D:482:VAL:HG13	2.03	0.40
1:A:94:LEU:C	1:A:96:LYS:H	2.25	0.40
1:A:243:ASN:ND2	1:A:246:ALA:HB2	2.36	0.40
1:B:28:ILE:O	1:B:28:ILE:HG22	2.22	0.40
1:B:311:SER:N	1:B:312:LYS:HB2	2.36	0.40
1:C:135:ILE:HG13	1:C:148:LEU:CD1	2.49	0.40
1:C:164:LEU:HD11	1:C:176:THR:HG21	2.03	0.40
1:C:395:SER:C	1:C:397:LEU:H	2.24	0.40
1:D:432:LEU:HD23	1:D:432:LEU:HA	1.88	0.40
1:A:264:ARG:HG2	1:A:370:ASN:CG	2.41	0.40
1:B:208:TYR:OH	1:B:357:LEU:N	2.52	0.40
1:A:264:ARG:HH22	1:A:372:LEU:H	1.66	0.40
1:B:91:SER:CA	1:B:92:SER:CB	2.99	0.40
1:D:88:ASP:CG	1:D:89:ASN:N	2.72	0.40
1:D:409:GLU:HA	1:D:411:ARG:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:SER:OG	1:D:412:GLU:OE2[4_555]	2.12	0.08

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	451/528 (85%)	386 (86%)	49 (11%)	16 (4%)	3	30
1	B	457/528 (87%)	380 (83%)	64 (14%)	13 (3%)	5	34
1	C	425/528 (80%)	376 (88%)	39 (9%)	10 (2%)	6	37
1	D	454/528 (86%)	393 (87%)	46 (10%)	15 (3%)	4	31
All	All	1787/2112 (85%)	1535 (86%)	198 (11%)	54 (3%)	4	33

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	B	266	GLU
1	B	415	THR
1	C	266	GLU
1	C	418	LEU
1	C	436	GLU
1	C	437	SER
1	D	34	SER
1	D	264	ARG
1	D	266	GLU
1	D	409	GLU
1	A	288	GLU
1	A	363	ALA
1	A	471	HIS
1	B	33	SER
1	B	38	GLU
1	B	264	ARG
1	B	313	PHE
1	B	335	ASN
1	B	352	LEU
1	B	361	VAL
1	C	85	GLY
1	C	104	GLY
1	D	37	PHE
1	A	85	GLY
1	A	261	ASN
1	A	311	SER
1	A	370	ASN
1	A	442	LEU
1	C	312	LYS
1	D	30	THR
1	D	123	ASN
1	D	308	LYS

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Mol	Chain	Res	Type
1	A	91	SER
1	A	165	GLN
1	A	310	VAL
1	B	127	PHE
1	C	93	VAL
1	D	85	GLY
1	D	247	THR
1	D	309	SER
1	A	95	ASN
1	A	309	SER
1	A	312	LYS
1	A	402	ALA
1	B	143	ASN
1	B	280	LYS
1	C	74	SER
1	D	104	GLY
1	D	133	GLN
1	D	213	GLY
1	D	246	ALA
1	B	67	ILE
1	C	67	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	365/470 (78%)	321 (88%)	44 (12%)	5 26
1	B	368/470 (78%)	319 (87%)	49 (13%)	4 23
1	C	328/470 (70%)	313 (95%)	15 (5%)	27 61
1	D	375/470 (80%)	334 (89%)	41 (11%)	6 32
All	All	1436/1880 (76%)	1287 (90%)	149 (10%)	7 34

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	28	ILE
1	A	40	THR
1	A	67	ILE
1	A	126	THR
1	A	131	THR
1	A	148	LEU
1	A	152	ASN
1	A	168	ASN
1	A	189	SER
1	A	190	LEU
1	A	236	ILE
1	A	240	ASN
1	A	241	ILE
1	A	250	LEU
1	A	275	THR
1	A	283	THR
1	A	285	THR
1	A	296	ILE
1	A	305	ASP
1	A	311	SER
1	A	321	LEU
1	A	343	VAL
1	A	349	ASP
1	A	352	LEU
1	A	365	ILE
1	A	372	LEU
1	A	376	VAL
1	A	392	LEU
1	A	393	VAL
1	A	397	LEU
1	A	404	SER
1	A	407	MET
1	A	413	PHE
1	A	424	SER
1	A	426	THR
1	A	436	GLU
1	A	437	SER
1	A	441	MET
1	A	445	ASP
1	A	450	SER
1	A	460	SER
1	A	464	THR

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Mol	Chain	Res	Type
1	A	476	ASP
1	B	30	THR
1	B	37	PHE
1	B	39	HIS
1	B	44	LEU
1	B	45	ASP
1	B	67	ILE
1	B	90	ILE
1	B	92	SER
1	B	117	SER
1	B	126	THR
1	B	156	THR
1	B	174	ILE
1	B	179	GLN
1	B	180	SER
1	B	184	ARG
1	B	185	ILE
1	B	221	ASN
1	B	236	ILE
1	B	242	ASP
1	B	265	CYS
1	B	272	THR
1	B	275	THR
1	B	311	SER
1	B	313	PHE
1	B	316	PHE
1	B	318	THR
1	B	329	LYS
1	B	332	GLN
1	B	338	ASP
1	B	340	GLU
1	B	344	ASN
1	B	347	THR
1	B	352	LEU
1	B	354	VAL
1	B	371	SER
1	B	374	ILE
1	B	382	LEU
1	B	387	THR
1	B	397	LEU
1	B	404	SER
1	B	416	VAL

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Mol	Chain	Res	Type
1	B	418	LEU
1	B	424	SER
1	B	434	ARG
1	B	438	ILE
1	B	444	LEU
1	B	445	ASP
1	B	448	THR
1	B	462	LYS
1	C	97	LEU
1	C	124	GLU
1	C	296	ILE
1	C	310	VAL
1	C	313	PHE
1	C	342	ILE
1	C	372	LEU
1	C	378	ARG
1	C	423	SER
1	C	430	ASP
1	C	436	GLU
1	C	445	ASP
1	C	448	THR
1	C	459	VAL
1	C	464	THR
1	D	33	SER
1	D	92	SER
1	D	106	LEU
1	D	126	THR
1	D	132	VAL
1	D	143	ASN
1	D	152	ASN
1	D	159	ASP
1	D	163	ILE
1	D	174	ILE
1	D	185	ILE
1	D	236	ILE
1	D	239	SER
1	D	242	ASP
1	D	243	ASN
1	D	247	THR
1	D	265	CYS
1	D	285	THR
1	D	296	ILE

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Mol	Chain	Res	Type
1	D	311	SER
1	D	322	TRP
1	D	324	SER
1	D	338	ASP
1	D	352	LEU
1	D	355	ILE
1	D	374	ILE
1	D	376	VAL
1	D	378	ARG
1	D	379	SER
1	D	393	VAL
1	D	399	SER
1	D	404	SER
1	D	415	THR
1	D	418	LEU
1	D	437	SER
1	D	438	ILE
1	D	441	MET
1	D	444	LEU
1	D	470	ASN
1	D	477	ILE
1	D	486	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	95	ASN
1	A	152	ASN
1	A	240	ASN
1	A	243	ASN
1	A	254	ASN
1	A	320	ASN
1	A	470	ASN
1	B	179	GLN
1	B	258	ASN
1	B	320	ASN
1	B	332	GLN
1	C	133	GLN
1	C	143	ASN
1	C	179	GLN
1	C	298	GLN

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Mol	Chain	Res	Type
1	D	39	HIS
1	D	95	ASN
1	D	103	ASN
1	D	143	ASN
1	D	179	GLN
1	D	254	ASN
1	D	370	ASN
1	D	458	ASN
1	D	470	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	457/528 (86%)	-0.46	2 (0%) 92 86	111, 166, 262, 329	0
1	B	463/528 (87%)	-0.57	1 (0%) 95 91	118, 155, 259, 321	0
1	C	439/528 (83%)	-0.16	17 (3%) 39 24	112, 243, 336, 404	0
1	D	460/528 (87%)	-0.65	0 100 100	102, 130, 188, 244	0
All	All	1819/2112 (86%)	-0.46	20 (1%) 80 66	102, 158, 293, 404	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	ASN	7.2
1	C	288	GLU	5.4
1	C	16	GLU	3.1
1	C	30	THR	2.9
1	C	265	CYS	2.8
1	C	349	ASP	2.8
1	C	336	ALA	2.7
1	C	169	HIS	2.7
1	C	283	THR	2.6
1	A	90	ILE	2.4
1	A	373	GLY	2.4
1	C	289	GLY	2.4
1	C	80	LYS	2.3
1	C	373	GLY	2.2
1	C	39	HIS	2.2
1	C	67	ILE	2.2
1	B	9	PHE	2.1
1	C	83	ALA	2.1
1	C	40	THR	2.1
1	C	369	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.