Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 AM GMT

PDB ID	:	2ZUN
Title	:	Functional Analysis of Hyperthermophilic Endocellulase from the Archaeon Pyrococcus horikoshii
Authors	:	Kim, H.-W.; Ishikawa, K.
Deposited on	:	2008-10-21
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

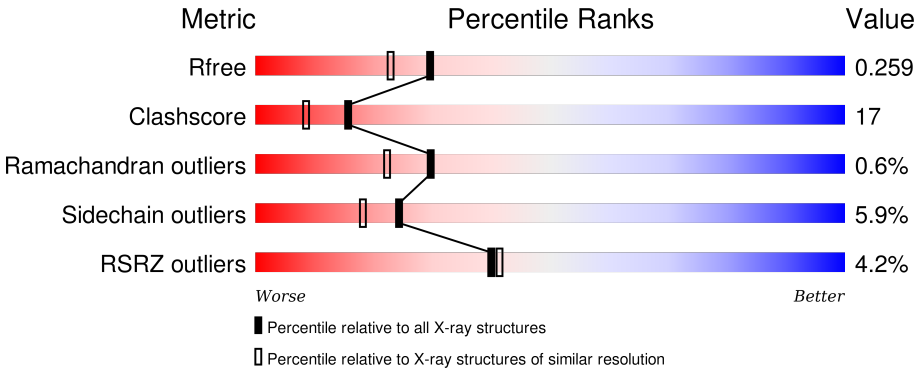
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	458	4% 60% 20% •• 18%
1	B	458	4% 58% 21% • 17%
1	C	458	3% 52% 26% 5% • 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CBI	A	459	X	-	-	X
2	CBI	B	459	X	-	-	X
2	CBI	B	460	-	-	-	X
2	CBI	C	459	X	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9875 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.

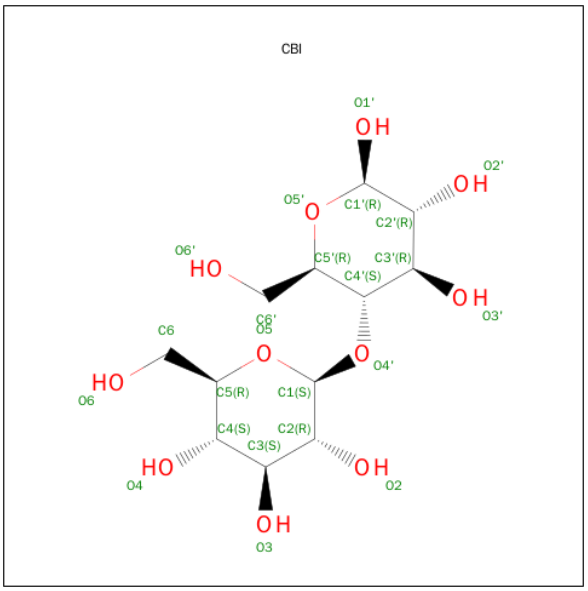
- Molecule 1 is a protein called 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			
1	B	379	Total	C	N	O	S	0	0	0
			3088	2015	502	561	10			
1	C	378	Total	C	N	O	S	0	0	0
			3081	2011	501	559	10			

There are 3 discrepancies between the modelled and reference sequences:

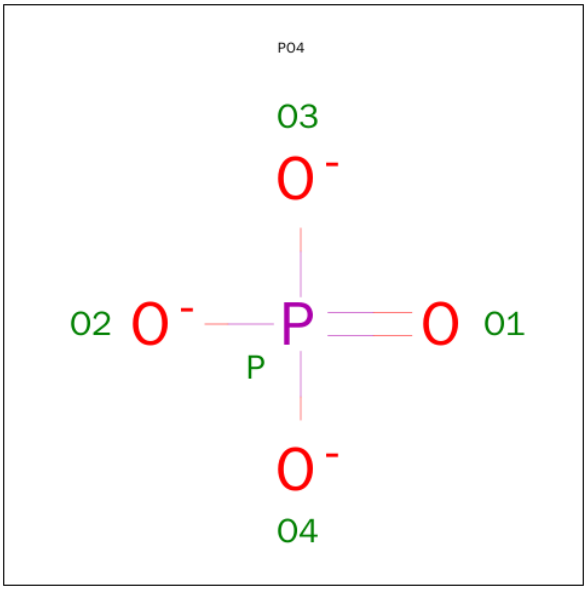
Chain	Residue	Modelled	Actual	Comment	Reference
A	289	LYS	ARG	SEE REMARK 999	UNP O58925
B	289	LYS	ARG	SEE REMARK 999	UNP O58925
C	289	LYS	ARG	SEE REMARK 999	UNP O58925

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 12 11	0	0
2	A	1	Total C O 23 12 11	0	0
2	B	1	Total C O 22 12 10	0	0
2	B	1	Total C O 23 12 11	0	0
2	C	1	Total C O 22 12 10	0	0
2	C	1	Total C O 23 12 11	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	193	Total O 193 193	0	0

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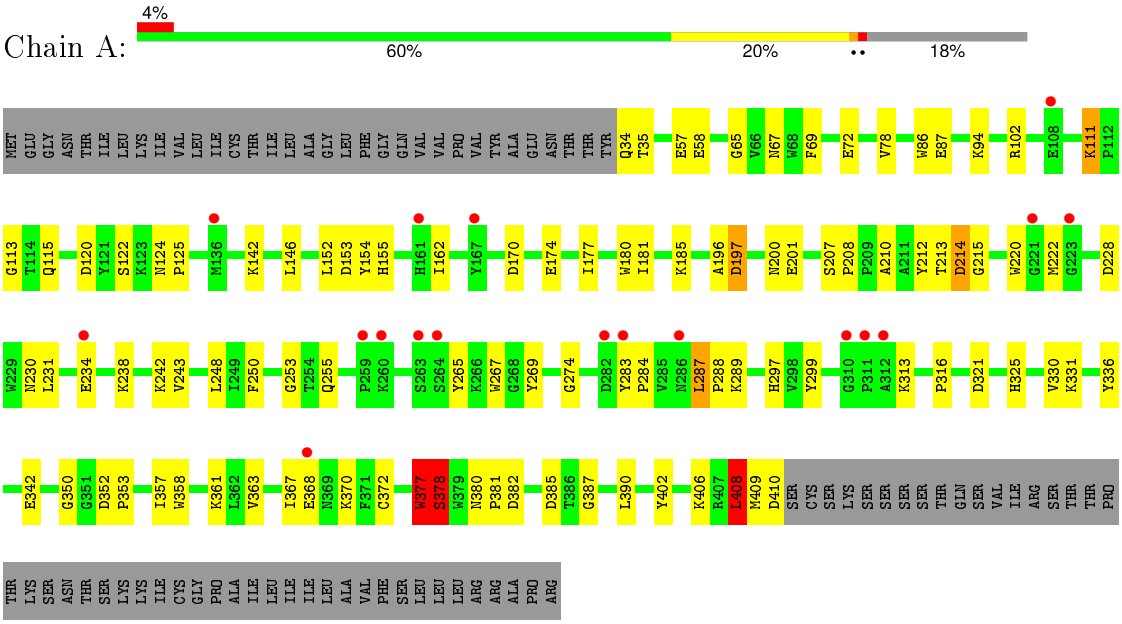
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	189	Total O 189 189	0	0
4	C	104	Total O 104 104	0	0

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.

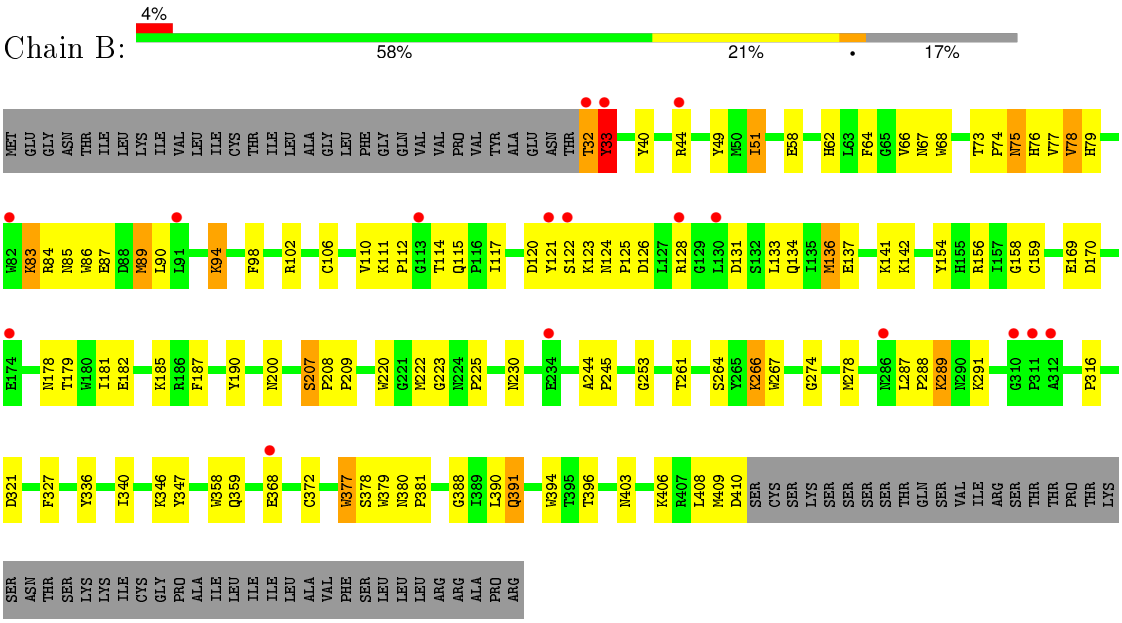
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain A:



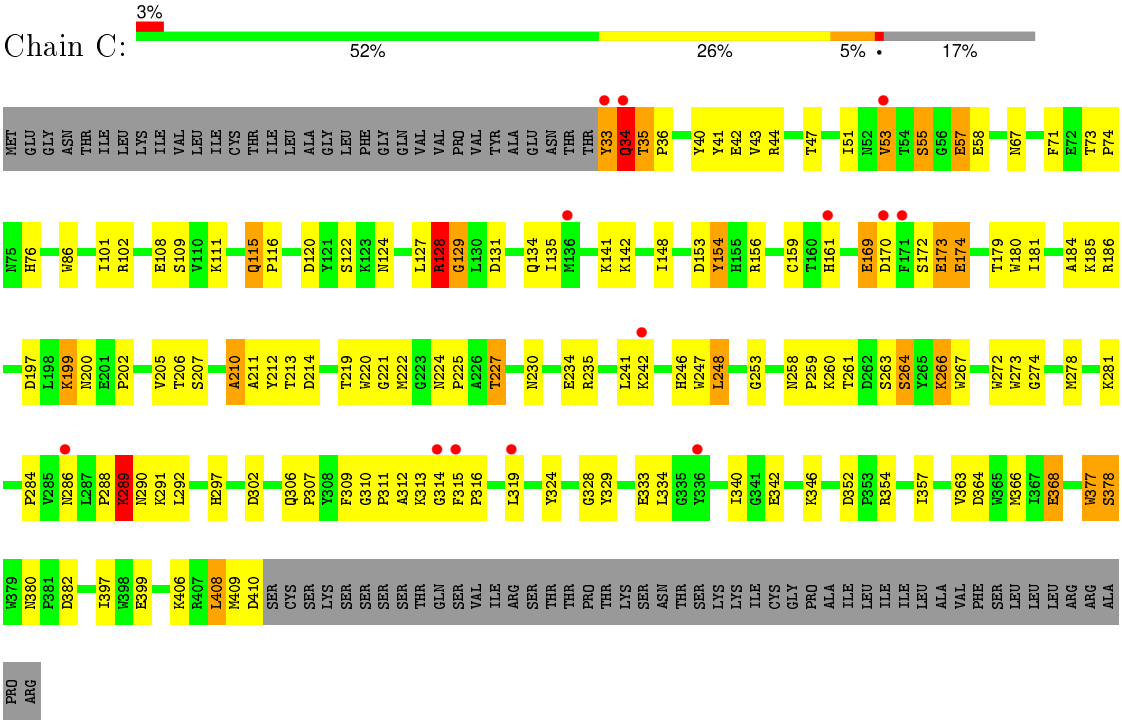
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain B:



• Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

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	162.16Å 58.40Å 138.33Å 90.00° 109.22° 90.00°	Depositor
Resolution (Å)	48.37 – 2.00 48.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.37-2.00) 98.0 (48.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.74 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.225 0.216 , 0.259	Depositor DCC
R_{free} test set	4075 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 81360 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9875	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: PO4, CBI

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	0.64	1/3180 (0.0%)	0.98	8/4341 (0.2%)
1	B	0.63	1/3200 (0.0%)	0.96	6/4369 (0.1%)
1	C	0.69	5/3193 (0.2%)	0.97	7/4359 (0.2%)
All	All	0.66	7/9573 (0.1%)	0.97	21/13069 (0.2%)

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	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	VAL	CA-CB	10.43	1.76	1.54
1	C	129	GLY	CA-C	-8.04	1.39	1.51
1	C	128	ARG	CA-C	-7.05	1.34	1.52
1	C	408	LEU	CB-CG	6.84	1.72	1.52
1	A	408	LEU	CB-CG	6.67	1.71	1.52
1	B	408	LEU	CB-CG	6.28	1.70	1.52
1	C	129	GLY	N-CA	-6.16	1.36	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	SER	N-CA-CB	-11.83	92.75	110.50
1	A	378	SER	N-CA-CB	11.20	127.30	110.50
1	A	408	LEU	CA-CB-CG	8.86	135.67	115.30
1	A	377	TRP	CA-C-N	-8.49	98.52	117.20
1	B	377	TRP	CA-C-N	-7.26	101.23	117.20
1	C	128	ARG	CA-C-N	-6.54	103.11	116.20
1	B	33	TYR	N-CA-C	6.35	128.15	111.00
1	B	378	SER	N-CA-C	6.17	127.65	111.00
1	C	378	SER	N-CA-CB	6.11	119.66	110.50
1	C	115	GLN	C-N-CD	6.11	141.22	128.40
1	C	197	ASP	N-CA-C	-6.09	94.55	111.00
1	A	197	ASP	N-CA-C	-5.87	95.17	111.00
1	C	278	MET	CA-CB-CG	5.74	123.06	113.30
1	B	377	TRP	CB-CA-C	5.72	121.84	110.40
1	B	377	TRP	N-CA-C	-5.66	95.72	111.00
1	A	65	GLY	N-CA-C	5.51	126.87	113.10
1	C	34	GLN	CA-CB-CG	5.50	125.50	113.40
1	C	129	GLY	N-CA-C	5.34	126.44	113.10
1	A	287	LEU	C-N-CD	5.33	139.60	128.40
1	A	387	GLY	N-CA-C	-5.22	100.05	113.10
1	A	113	GLY	N-CA-C	5.14	125.95	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	TRP	Mainchain,Peptide
1	B	377	TRP	Mainchain,Peptide
1	C	377	TRP	Mainchain,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	3069	0	2910	79	0
1	B	3088	0	2926	110	0
1	C	3081	0	2919	120	0
2	A	46	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	45	0	39	0	0
2	C	45	0	39	5	0
3	A	15	0	0	0	0
4	A	193	0	0	14	1
4	B	189	0	0	20	0
4	C	104	0	0	5	0
All	All	9875	0	8876	311	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 (311) 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:53:VAL:CB	1:C:53:VAL:CA	1.76	1.58
1:A:212:TYR:HB3	1:A:222:MET:CE	1.75	1.16
1:A:212:TYR:HB3	1:A:222:MET:HE2	1.14	1.11
1:C:266:LYS:H	1:C:266:LYS:HD2	1.05	1.10
1:A:34:GLN:HA	4:A:472:HOH:O	1.56	1.05
1:A:111:LYS:HZ2	1:A:111:LYS:HB3	1.29	0.98
1:C:128:ARG:HD2	4:C:462:HOH:O	1.63	0.98
1:C:333:GLU:HG2	1:C:334:LEU:HD23	1.45	0.96
1:A:111:LYS:NZ	1:A:111:LYS:HB3	1.81	0.95
1:B:372:CYS:HB2	4:B:483:HOH:O	1.68	0.92
1:C:289:LYS:O	1:C:289:LYS:HG3	1.66	0.92
1:B:133:LEU:HG	4:B:643:HOH:O	1.69	0.91
1:B:131:ASP:OD1	1:B:134:GLN:HG3	1.71	0.89
1:C:266:LYS:N	1:C:266:LYS:HD2	1.84	0.89
1:B:131:ASP:OD1	1:B:134:GLN:CG	2.22	0.88
1:C:406:LYS:HA	1:C:409:MET:HE2	1.57	0.87
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.23	0.86
1:C:173:GLU:HG3	1:C:173:GLU:O	1.72	0.86
1:B:136:MET:HE2	1:B:187:PHE:CZ	2.11	0.86
1:A:212:TYR:CB	1:A:222:MET:HE2	2.05	0.84
1:B:136:MET:CE	1:B:187:PHE:CZ	2.60	0.83
1:C:169:GLU:HG3	1:C:170:ASP:N	1.93	0.83
1:C:76:HIS:HE1	1:C:159:CYS:SG	2.01	0.83
1:B:261:THR:O	1:B:264:SER:OG	1.97	0.82
1:B:134:GLN:HG3	4:B:637:HOH:O	1.79	0.81
1:B:51:ILE:HD13	1:B:58:GLU:HG2	1.61	0.81
1:A:410:ASP:HB3	4:A:632:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.28	0.79
1:C:53:VAL:CB	1:C:53:VAL:C	2.51	0.79
1:B:83:LYS:O	1:B:83:LYS:HD3	1.82	0.79
1:B:67:ASN:HD21	1:B:102:ARG:HD3	1.46	0.79
1:A:234:GLU:HB2	4:A:641:HOH:O	1.83	0.78
1:A:87:GLU:OE2	1:A:142:LYS:HE3	1.84	0.77
1:C:311:PRO:O	1:C:313:LYS:N	2.18	0.77
1:C:333:GLU:HG2	1:C:334:LEU:CD2	2.14	0.76
1:B:33:TYR:H	1:B:33:TYR:HD1	1.32	0.76
1:C:71:PHE:O	1:C:109:SER:OG	2.05	0.75
1:A:242:LYS:HE2	4:A:644:HOH:O	1.86	0.75
1:C:281:LYS:HB3	1:C:281:LYS:HZ1	1.52	0.74
1:A:120:ASP:OD1	1:A:122:SER:HB3	1.86	0.74
1:C:334:LEU:N	1:C:334:LEU:HD23	2.02	0.74
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.36	0.73
1:C:281:LYS:CB	1:C:281:LYS:NZ	2.48	0.72
1:B:74:PRO:HD3	1:B:159:CYS:O	1.90	0.72
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.38	0.72
1:A:361:LYS:HD2	4:A:616:HOH:O	1.90	0.71
1:C:67:ASN:ND2	1:C:102:ARG:HH11	1.87	0.71
1:C:186:ARG:HH11	1:C:186:ARG:HG3	1.56	0.71
1:A:177:ILE:HG22	1:A:181:ILE:HD12	1.72	0.71
1:C:281:LYS:NZ	1:C:281:LYS:HB3	2.04	0.70
1:B:372:CYS:CB	4:B:483:HOH:O	2.34	0.70
1:C:309:PHE:O	1:C:311:PRO:HD3	1.91	0.70
2:C:459:CBI:H6'1	2:C:460:CBI:O1'	1.92	0.70
1:C:368:GLU:C	1:C:368:GLU:OE2	2.30	0.69
1:C:206:THR:OG1	1:C:214:ASP:OD2	2.11	0.69
1:C:267:TRP:CZ3	1:C:307:PRO:HB2	2.28	0.68
1:A:253:GLY:O	1:A:274:GLY:HA2	1.94	0.68
1:A:385:ASP:HB3	4:A:648:HOH:O	1.94	0.67
1:A:212:TYR:HB3	1:A:222:MET:HE1	1.72	0.67
1:C:120:ASP:OD1	1:C:122:SER:HB3	1.94	0.67
1:C:409:MET:O	1:C:410:ASP:HB2	1.93	0.67
1:B:84:ARG:NH1	1:B:394:TRP:O	2.26	0.67
1:B:340:ILE:HG13	4:B:486:HOH:O	1.94	0.66
1:B:381:PRO:HD2	1:B:394:TRP:CZ2	2.30	0.66
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.41	0.66
1:A:34:GLN:CA	4:A:472:HOH:O	2.29	0.66
1:C:33:TYR:HD1	1:C:34:GLN:N	1.94	0.66
1:A:94:LYS:NZ	1:A:146:LEU:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.32	0.65
1:B:110:VAL:HA	1:B:133:LEU:HD13	1.79	0.64
1:B:379:TRP:CE2	1:B:390:LEU:HD11	2.32	0.64
1:A:86:TRP:H	1:A:124:ASN:HD21	1.43	0.64
1:C:34:GLN:C	1:C:35:THR:HG22	2.18	0.64
1:C:35:THR:HB	1:C:246:HIS:HB3	1.78	0.64
1:A:86:TRP:HD1	1:A:124:ASN:HD22	1.45	0.64
1:C:86:TRP:H	1:C:124:ASN:HD21	1.45	0.64
1:B:209:PRO:HD2	4:B:633:HOH:O	1.96	0.64
1:C:342:GLU:OE1	2:C:459:CBI:C1'	2.46	0.64
1:C:53:VAL:CG1	1:C:53:VAL:CA	2.74	0.63
1:B:74:PRO:O	1:B:76:HIS:CD2	2.52	0.63
1:B:75:ASN:HA	1:B:117:ILE:HG12	1.81	0.62
1:C:53:VAL:CG2	1:C:53:VAL:CA	2.74	0.62
1:C:55:SER:HB2	1:C:57:GLU:HB2	1.79	0.62
1:C:186:ARG:HG3	1:C:186:ARG:NH1	2.13	0.62
2:C:459:CBI:H4'	4:C:482:HOH:O	2.00	0.62
1:C:311:PRO:C	1:C:313:LYS:H	2.03	0.61
1:A:102:ARG:HH22	1:A:200:ASN:ND2	1.98	0.61
1:B:136:MET:HE2	1:B:187:PHE:HZ	1.62	0.61
1:B:83:LYS:C	1:B:83:LYS:HD3	2.16	0.61
1:A:212:TYR:CB	1:A:222:MET:CE	2.67	0.61
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.66	0.61
1:C:281:LYS:O	1:C:284:PRO:HD3	2.01	0.61
1:B:87:GLU:CB	4:B:648:HOH:O	2.49	0.60
1:B:87:GLU:HB2	4:B:648:HOH:O	1.99	0.60
1:B:86:TRP:HD1	1:B:124:ASN:ND2	1.99	0.60
1:B:86:TRP:H	1:B:124:ASN:ND2	1.99	0.60
1:B:121:TYR:CD1	1:B:128:ARG:HG2	2.37	0.60
1:B:131:ASP:OD1	1:B:134:GLN:HG2	2.01	0.60
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.50	0.60
1:C:352:ASP:OD1	1:C:354:ARG:HB2	2.02	0.60
1:A:297:HIS:CE1	1:A:342:GLU:HG3	2.37	0.60
1:C:76:HIS:CE1	1:C:159:CYS:SG	2.90	0.59
1:B:44:ARG:HG3	1:B:49:TYR:CD2	2.36	0.59
1:B:64:PHE:CD2	1:B:409:MET:HG2	2.37	0.59
1:B:266:LYS:HE2	1:B:267:TRP:NE1	2.15	0.59
1:B:86:TRP:O	1:B:89:MET:HB2	2.02	0.59
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.38	0.59
1:A:212:TYR:OH	1:A:269:TYR:HE1	1.86	0.58
1:A:67:ASN:ND2	1:A:102:ARG:HH11	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:SER:O	1:A:210:ALA:HB3	2.04	0.58
1:C:364:ASP:O	1:C:368:GLU:HG3	2.04	0.57
1:A:234:GLU:O	1:A:238:LYS:HG3	2.04	0.57
1:B:170:ASP:HB2	4:B:631:HOH:O	2.03	0.57
1:B:68:TRP:CZ2	1:B:89:MET:HG3	2.39	0.57
1:B:90:LEU:HD12	1:B:142:LYS:CG	2.34	0.57
1:C:281:LYS:CB	1:C:281:LYS:HZ1	2.12	0.57
1:A:255:GLN:HB3	4:A:477:HOH:O	2.04	0.57
1:B:223:GLY:O	1:B:225:PRO:HD3	2.05	0.56
1:C:221:GLY:HA2	4:C:557:HOH:O	2.04	0.56
1:B:86:TRP:CZ3	4:B:648:HOH:O	2.53	0.56
1:C:272:TRP:HE3	2:C:460:CBI:H6'1	1.70	0.56
1:A:331:LYS:HE3	1:A:370:LYS:O	2.05	0.56
1:C:169:GLU:HG3	1:C:170:ASP:H	1.66	0.56
1:B:67:ASN:ND2	1:B:102:ARG:HH11	2.03	0.56
1:B:381:PRO:HD2	1:B:394:TRP:CH2	2.41	0.55
1:C:222:MET:SD	1:C:259:PRO:HD3	2.46	0.55
1:B:253:GLY:O	1:B:274:GLY:HA2	2.07	0.55
1:B:289:LYS:HE2	1:B:336:TYR:CE2	2.42	0.55
1:A:86:TRP:H	1:A:124:ASN:ND2	2.05	0.55
1:A:316:PRO:HG3	1:A:357:ILE:CG2	2.37	0.55
1:B:32:THR:HA	1:B:40:TYR:CD2	2.42	0.55
1:A:380:ASN:HB3	1:A:382:ASP:OD1	2.06	0.55
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.54	0.54
1:B:106:CYS:SG	1:B:159:CYS:SG	3.02	0.54
1:B:391:GLN:HG3	1:B:396:THR:O	2.07	0.54
1:B:141:LYS:HD2	4:B:478:HOH:O	2.07	0.54
1:C:266:LYS:CD	1:C:266:LYS:H	1.97	0.54
1:C:44:ARG:NH1	1:C:58:GLU:OE1	2.37	0.53
1:B:73:THR:HB	1:B:74:PRO:HD2	1.89	0.53
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.73	0.53
1:A:287:LEU:O	1:A:288:PRO:C	2.46	0.53
1:C:258:ASN:ND2	1:C:261:THR:OG1	2.42	0.53
1:B:114:THR:HG22	1:B:115:GLN:N	2.24	0.52
1:C:86:TRP:H	1:C:124:ASN:ND2	2.07	0.52
1:C:131:ASP:OD1	1:C:134:GLN:HG3	2.10	0.52
1:B:111:LYS:O	1:B:112:PRO:C	2.44	0.52
1:A:350:GLY:HA2	4:A:484:HOH:O	2.09	0.52
1:A:111:LYS:NZ	1:A:111:LYS:CB	2.58	0.52
1:B:122:SER:O	1:B:125:PRO:HD3	2.09	0.52
1:B:178:ASN:O	1:B:182:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:HG22	1:B:78:VAL:N	2.25	0.52
1:C:241:LEU:O	1:C:242:LYS:C	2.46	0.52
1:A:34:GLN:N	4:A:472:HOH:O	2.42	0.52
1:B:86:TRP:CH2	4:B:648:HOH:O	2.63	0.51
1:B:133:LEU:O	1:B:136:MET:HB2	2.10	0.51
1:C:363:VAL:HG13	1:C:408:LEU:HB2	1.92	0.51
1:A:207:SER:HB3	1:A:208:PRO:HD2	1.91	0.51
1:C:311:PRO:HA	1:C:315:PHE:HB3	1.91	0.51
1:C:316:PRO:HG3	1:C:357:ILE:HG21	1.93	0.51
1:C:234:GLU:HG2	1:C:286:ASN:O	2.11	0.51
1:A:368:GLU:HG3	4:A:517:HOH:O	2.11	0.50
1:B:409:MET:O	1:B:410:ASP:HB2	2.10	0.50
1:C:316:PRO:O	1:C:319:LEU:HG	2.11	0.50
1:B:379:TRP:CZ2	1:B:390:LEU:HD11	2.46	0.50
1:C:212:TYR:HB3	1:C:222:MET:HE1	1.93	0.50
1:B:179:THR:O	1:B:182:GLU:HG3	2.12	0.50
1:A:367:ILE:HG13	1:A:408:LEU:HD13	1.93	0.50
1:C:156:ARG:HG2	1:C:161:HIS:O	2.12	0.50
1:B:86:TRP:N	1:B:124:ASN:HD21	2.10	0.50
1:B:409:MET:O	1:B:410:ASP:CB	2.60	0.50
1:A:377:TRP:C	1:A:377:TRP:CD1	2.86	0.49
1:A:352:ASP:OD1	1:A:353:PRO:HD2	2.12	0.49
1:A:409:MET:O	1:A:410:ASP:HB2	2.12	0.49
1:B:114:THR:CG2	1:B:115:GLN:N	2.75	0.49
1:C:108:GLU:HB2	4:C:486:HOH:O	2.12	0.49
1:B:85:ASN:HA	1:B:124:ASN:ND2	2.28	0.49
1:B:67:ASN:ND2	1:B:102:ARG:HD3	2.22	0.49
1:C:324:TYR:CE2	1:C:329:TYR:HB3	2.47	0.49
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.61	0.49
1:C:210:ALA:O	1:C:214:ASP:HB3	2.13	0.49
1:B:207:SER:CB	1:B:208:PRO:HD2	2.43	0.48
1:C:116:PRO:HG3	1:C:135:ILE:HD12	1.95	0.48
1:B:278:MET:O	4:B:549:HOH:O	2.20	0.48
1:B:74:PRO:O	1:B:76:HIS:HD2	1.94	0.48
1:C:219:THR:HG21	1:C:222:MET:HG3	1.96	0.48
1:B:123:LYS:C	1:B:125:PRO:HD3	2.34	0.48
1:C:267:TRP:HZ3	1:C:307:PRO:HB2	1.77	0.48
1:C:55:SER:C	1:C:57:GLU:H	2.16	0.48
1:C:291:LYS:HE2	1:C:291:LYS:HA	1.95	0.48
1:C:340:ILE:HD12	1:C:366:MET:HE3	1.96	0.48
1:B:124:ASN:N	1:B:125:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:VAL:CB	1:C:53:VAL:O	2.61	0.47
1:B:391:GLN:HG3	1:B:396:THR:HB	1.95	0.47
1:C:73:THR:HB	1:C:74:PRO:CD	2.44	0.47
1:C:41:TYR:HB3	1:C:248:LEU:HD21	1.95	0.47
1:A:321:ASP:OD1	1:A:325:HIS:CE1	2.67	0.47
1:B:86:TRP:H	1:B:124:ASN:HD21	1.60	0.47
1:C:42:GLU:OE1	1:C:51:ILE:HD11	2.15	0.47
1:B:346:LYS:O	1:B:347:TYR:C	2.52	0.47
1:A:162:ILE:HD11	2:A:459:CBI:H2'	1.94	0.47
1:C:200:ASN:ND2	1:C:297:HIS:HE1	2.13	0.47
1:A:200:ASN:ND2	1:A:201:GLU:HG3	2.29	0.47
1:B:368:GLU:HG3	4:B:504:HOH:O	2.15	0.47
1:C:397:ILE:HG12	4:C:516:HOH:O	2.14	0.47
1:C:181:ILE:CG2	1:C:185:LYS:HE3	2.45	0.47
1:C:235:ARG:HG3	1:C:235:ARG:HH11	1.79	0.47
1:A:180:TRP:CH2	1:A:196:ALA:HB1	2.50	0.47
1:C:264:SER:OG	1:C:264:SER:O	2.27	0.47
1:B:190:TYR:CD2	1:B:190:TYR:N	2.83	0.46
1:B:136:MET:CE	1:B:187:PHE:CE2	2.98	0.46
1:A:228:ASP:HB3	1:A:231:LEU:HG	1.98	0.46
1:A:86:TRP:N	1:A:124:ASN:HD21	2.13	0.46
1:C:35:THR:HB	1:C:246:HIS:CB	2.44	0.46
1:C:127:LEU:O	1:C:129:GLY:N	2.49	0.46
1:A:213:THR:O	1:A:215:GLY:N	2.49	0.46
1:C:340:ILE:HD12	1:C:366:MET:CE	2.45	0.46
1:C:311:PRO:O	1:C:314:GLY:N	2.48	0.46
1:A:299:TYR:OH	1:A:342:GLU:OE1	2.27	0.46
1:C:181:ILE:HG23	1:C:185:LYS:HE3	1.99	0.45
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.51	0.45
1:B:90:LEU:HD12	1:B:142:LYS:HG3	1.98	0.45
1:C:302:ASP:OD2	1:C:346:LYS:HB2	2.16	0.45
1:A:361:LYS:CD	4:A:616:HOH:O	2.57	0.45
1:A:69:PHE:HB2	1:A:72:GLU:OE2	2.16	0.45
1:B:64:PHE:CG	1:B:409:MET:HG2	2.51	0.45
1:A:197:ASP:HA	1:A:250:PHE:HB2	1.98	0.45
1:B:133:LEU:O	1:B:137:GLU:HG3	2.17	0.45
1:B:86:TRP:CE3	4:B:648:HOH:O	2.70	0.45
1:C:316:PRO:HG3	1:C:357:ILE:CG2	2.46	0.45
1:C:154:TYR:CZ	1:C:179:THR:HG21	2.51	0.45
1:B:380:ASN:O	1:B:388:GLY:HA3	2.16	0.45
1:C:115:GLN:NE2	1:C:116:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ASP:OD2	1:B:123:LYS:HD2	2.17	0.44
1:C:311:PRO:C	1:C:313:LYS:N	2.64	0.44
1:B:287:LEU:HB3	1:B:288:PRO:HD2	1.98	0.44
1:A:299:TYR:C	1:A:358:TRP:CZ2	2.91	0.44
1:B:181:ILE:O	1:B:185:LYS:HG3	2.18	0.44
1:B:136:MET:HE3	1:B:136:MET:HB3	1.93	0.44
1:C:310:GLY:O	1:C:311:PRO:C	2.55	0.44
1:C:206:THR:O	1:C:211:ALA:HB2	2.18	0.44
1:C:36:PRO:HD2	1:C:246:HIS:CE1	2.52	0.44
1:B:291:LYS:HA	1:B:291:LYS:HE2	1.99	0.44
1:C:224:ASN:HA	1:C:225:PRO:HD2	1.53	0.44
1:C:33:TYR:CD1	1:C:34:GLN:HG2	2.52	0.44
1:A:381:PRO:HD3	1:A:390:LEU:HB2	1.99	0.44
1:B:87:GLU:CD	1:B:142:LYS:HE3	2.38	0.44
1:A:381:PRO:HB3	1:A:390:LEU:O	2.18	0.44
1:C:253:GLY:O	1:C:274:GLY:HA2	2.17	0.44
1:C:406:LYS:HG3	1:C:409:MET:CE	2.47	0.43
1:B:76:HIS:CE1	4:B:508:HOH:O	2.71	0.43
1:A:377:TRP:HA	1:A:378:SER:HA	1.84	0.43
1:C:184:ALA:HA	1:C:247:TRP:CH2	2.53	0.43
1:B:321:ASP:HB3	4:B:524:HOH:O	2.18	0.43
1:A:283:TYR:N	1:A:284:PRO:CD	2.80	0.43
1:A:207:SER:HB3	1:A:208:PRO:CD	2.48	0.43
1:C:219:THR:OG1	1:C:227:THR:OG1	2.17	0.43
1:A:363:VAL:HG13	1:A:408:LEU:HD22	2.00	0.43
1:A:208:PRO:HB3	1:A:212:TYR:CE2	2.54	0.43
1:C:241:LEU:HD23	1:C:241:LEU:HA	1.71	0.43
1:B:66:VAL:HG13	1:B:98:PHE:CD1	2.53	0.43
1:A:174:GLU:O	1:A:174:GLU:HG2	2.19	0.43
1:A:265:TYR:CE2	1:A:267:TRP:HB2	2.53	0.43
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.15	0.43
1:A:155:HIS:HA	1:A:200:ASN:CB	2.49	0.43
1:A:402:TYR:CE2	1:A:406:LYS:HD2	2.54	0.43
1:B:316:PRO:HD2	4:B:625:HOH:O	2.19	0.43
1:C:306:GLN:HB2	1:C:309:PHE:CD2	2.54	0.43
1:B:62:HIS:CD2	1:B:62:HIS:O	2.72	0.42
1:B:75:ASN:N	1:B:75:ASN:OD1	2.51	0.42
1:B:381:PRO:HD2	1:B:394:TRP:CE2	2.55	0.42
1:A:152:LEU:HA	1:A:152:LEU:HD23	1.93	0.42
1:C:101:ILE:HD12	1:C:148:ILE:HG21	2.00	0.42
1:A:330:VAL:HG12	1:A:336:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HG13	1:A:408:LEU:CD1	2.50	0.42
1:C:172:SER:C	1:C:174:GLU:N	2.73	0.42
1:B:126:ASP:OD1	1:B:126:ASP:N	2.53	0.42
1:A:162:ILE:CD1	2:A:459:CBI:H2'	2.49	0.42
1:A:372:CYS:HA	4:A:509:HOH:O	2.19	0.42
1:A:177:ILE:HG22	1:A:181:ILE:CD1	2.45	0.42
1:B:111:LYS:HA	1:B:111:LYS:HD3	1.92	0.42
1:B:156:ARG:HB3	1:B:158:GLY:O	2.20	0.42
1:B:121:TYR:CE1	1:B:128:ARG:HA	2.55	0.42
1:C:212:TYR:O	1:C:222:MET:HE2	2.19	0.42
1:B:94:LYS:O	1:B:94:LYS:HE3	2.20	0.42
1:C:377:TRP:HA	1:C:378:SER:HA	1.81	0.42
1:C:33:TYR:CD1	1:C:34:GLN:N	2.81	0.41
1:B:358:TRP:CE3	1:B:359:GLN:HG2	2.55	0.41
1:B:137:GLU:CD	4:B:643:HOH:O	2.59	0.41
1:B:90:LEU:CD1	1:B:142:LYS:HG3	2.49	0.41
1:B:79:HIS:HA	4:B:471:HOH:O	2.20	0.41
1:C:86:TRP:N	1:C:124:ASN:HD21	2.15	0.41
1:A:214:ASP:C	1:A:214:ASP:OD2	2.58	0.41
1:C:329:TYR:O	1:C:333:GLU:HB3	2.20	0.41
1:A:57:GLU:HG3	1:A:58:GLU:N	2.34	0.41
1:B:89:MET:CE	1:B:394:TRP:CE3	3.03	0.41
1:A:94:LYS:HE3	4:A:655:HOH:O	2.20	0.41
1:B:406:LYS:HA	1:B:409:MET:CE	2.51	0.41
1:A:248:LEU:HA	1:A:248:LEU:HD23	1.80	0.41
1:C:273:TRP:CE2	2:C:460:CBI:H4'	2.55	0.41
1:C:40:TYR:HA	1:C:246:HIS:HB2	2.02	0.41
1:B:244:ALA:N	1:B:245:PRO:CD	2.83	0.41
1:B:90:LEU:HD12	1:B:142:LYS:HG2	2.02	0.41
1:C:43:VAL:HG12	1:C:44:ARG:N	2.34	0.41
1:C:380:ASN:HB3	1:C:382:ASP:OD1	2.21	0.41
1:C:199:LYS:HD3	1:C:202:PRO:HD3	2.03	0.41
1:B:76:HIS:ND1	1:B:114:THR:HG21	2.36	0.41
1:C:51:ILE:HG12	1:C:58:GLU:HB2	2.02	0.40
1:C:142:LYS:HA	1:C:142:LYS:HD3	1.85	0.40
1:C:324:TYR:HA	1:C:328:GLY:HA3	2.03	0.40
1:C:33:TYR:C	1:C:33:TYR:HD1	2.24	0.40
1:C:288:PRO:O	1:C:290:ASN:N	2.54	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)
4:A:558:HOH:O	4:A:558:HOH:O[2_555]	1.84	0.36

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	375/458 (82%)	359 (96%)	14 (4%)	2 (0%)	34 26
1	B	377/458 (82%)	362 (96%)	14 (4%)	1 (0%)	46 41
1	C	376/458 (82%)	345 (92%)	27 (7%)	4 (1%)	17 9
All	All	1128/1374 (82%)	1066 (94%)	55 (5%)	7 (1%)	30 22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	312	ALA
1	C	289	LYS
1	A	214	ASP
1	C	128	ARG
1	C	210	ALA
1	A	378	SER
1	B	327	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/396 (82%)	311 (96%)	13 (4%)	38 33
1	B	326/396 (82%)	309 (95%)	17 (5%)	29 23
1	C	325/396 (82%)	297 (91%)	28 (9%)	13 7
All	All	975/1188 (82%)	917 (94%)	58 (6%)	24 18

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	78	VAL
1	A	111	LYS
1	A	115	GLN
1	A	125	PRO
1	A	153	ASP
1	A	154	TYR
1	A	170	ASP
1	A	185	LYS
1	A	243	VAL
1	A	289	LYS
1	A	313	LYS
1	A	408	LEU
1	B	32	THR
1	B	33	TYR
1	B	51	ILE
1	B	75	ASN
1	B	78	VAL
1	B	83	LYS
1	B	89	MET
1	B	94	LYS
1	B	136	MET
1	B	154	TYR
1	B	169	GLU
1	B	207	SER
1	B	222	MET
1	B	266	LYS
1	B	289	LYS
1	B	391	GLN
1	B	403	ASN
1	C	33	TYR

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Mol	Chain	Res	Type
1	C	34	GLN
1	C	35	THR
1	C	47	THR
1	C	55	SER
1	C	57	GLU
1	C	111	LYS
1	C	141	LYS
1	C	153	ASP
1	C	154	TYR
1	C	169	GLU
1	C	173	GLU
1	C	174	GLU
1	C	180	TRP
1	C	199	LYS
1	C	205	VAL
1	C	207	SER
1	C	213	THR
1	C	227	THR
1	C	248	LEU
1	C	260	LYS
1	C	263	SER
1	C	264	SER
1	C	266	LYS
1	C	289	LYS
1	C	292	LEU
1	C	368	GLU
1	C	399	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	67	ASN
1	A	76	HIS
1	A	115	GLN
1	A	124	ASN
1	A	200	ASN
1	A	359	GLN
1	B	62	HIS
1	B	67	ASN
1	B	76	HIS
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	200	ASN
1	B	359	GLN
1	C	67	ASN
1	C	76	HIS
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	359	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CBI	A	459	-	24,24,24	0.46	0	35,35,35	3.66	21 (60%)
2	CBI	A	460	-	24,24,24	0.47	0	35,35,35	3.55	22 (62%)
3	PO4	A	461	-	4,4,4	1.64	1 (25%)	6,6,6	0.27	0
3	PO4	A	462	-	4,4,4	1.57	1 (25%)	6,6,6	0.27	0
3	PO4	A	463	-	4,4,4	1.57	1 (25%)	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CBI	B	459	-	23,23,24	0.47	0	33,33,35	4.06	20 (60%)
2	CBI	B	460	-	24,24,24	0.60	0	35,35,35	2.99	19 (54%)
2	CBI	C	459	-	23,23,24	0.45	0	33,33,35	3.63	19 (57%)
2	CBI	C	460	-	24,24,24	0.48	0	35,35,35	4.05	21 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBI	A	459	-	1/1/10/10	0/8/48/48	0/2/2/2
2	CBI	A	460	-	-	0/8/48/48	0/2/2/2
3	PO4	A	461	-	-	0/0/0/0	0/0/0/0
3	PO4	A	462	-	-	0/0/0/0	0/0/0/0
3	PO4	A	463	-	-	0/0/0/0	0/0/0/0
2	CBI	B	459	-	2/2/9/10	0/8/45/48	0/2/2/2
2	CBI	B	460	-	-	0/8/48/48	0/2/2/2
2	CBI	C	459	-	1/1/9/10	0/8/45/48	0/2/2/2
2	CBI	C	460	-	-	0/8/48/48	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	461	PO4	P-O2	-2.55	1.44	1.53
3	A	462	PO4	P-O4	-2.28	1.45	1.53
3	A	463	PO4	P-O2	-2.15	1.45	1.53

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	459	CBI	O4'-C4'-C5'	-10.78	81.00	109.32
2	C	460	CBI	C1-O5-C5	-10.09	94.17	113.75
2	A	459	CBI	C1-O5-C5	-9.83	94.67	113.75
2	C	460	CBI	C3-C4-C5	-9.48	93.67	110.20
2	C	460	CBI	C1'-O5'-C5'	-7.71	99.20	113.47
2	C	460	CBI	C3'-C4'-C5'	-7.64	93.57	110.84
2	A	460	CBI	C1'-C2'-C3'	-7.56	99.18	110.43
2	A	460	CBI	O4-C4-C3	-7.43	93.60	110.34
2	A	460	CBI	O4'-C4'-C5'	-7.43	89.79	109.32
2	A	459	CBI	O4-C4-C3	-7.33	93.84	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	459	CBI	O4'-C4'-C5'	-7.27	90.22	109.32
2	B	459	CBI	O2-C2-C3	-6.88	94.85	110.34
2	B	460	CBI	O4-C4-C3	-6.61	95.46	110.34
2	A	459	CBI	O4'-C4'-C3'	-6.56	90.24	107.17
2	B	460	CBI	C3-C4-C5	-6.27	99.27	110.20
2	A	460	CBI	O4-C4-C5	-6.02	93.28	109.24
2	B	459	CBI	O4-C4-C3	-5.80	97.29	110.34
2	C	460	CBI	O4-C4-C3	-5.73	97.45	110.34
2	C	459	CBI	C3-C4-C5	-5.68	100.30	110.20
2	A	460	CBI	O4'-C4'-C3'	-5.65	92.59	107.17
2	B	459	CBI	C3'-C4'-C5'	-5.35	98.73	110.84
2	B	459	CBI	O4-C4-C5	-5.32	95.15	109.24
2	C	460	CBI	O2-C2-C3	-5.16	98.72	110.34
2	B	460	CBI	C1'-O5'-C5'	-5.14	103.97	113.47
2	C	460	CBI	O4'-C4'-C3'	-5.07	94.09	107.17
2	C	459	CBI	C1'-C2'-C3'	-4.84	103.81	109.54
2	B	460	CBI	O4'-C4'-C5'	-4.70	96.97	109.32
2	B	460	CBI	C1-O5-C5	-4.54	104.93	113.75
2	B	460	CBI	C3'-C4'-C5'	-4.52	100.61	110.84
2	B	459	CBI	O4'-C1-O5	-4.46	99.39	110.68
2	B	459	CBI	O5'-C1'-C2'	-4.36	103.78	110.86
2	C	460	CBI	O4'-C4'-C5'	-4.25	98.16	109.32
2	A	459	CBI	C3'-C4'-C5'	-4.06	101.67	110.84
2	C	460	CBI	C1'-C2'-C3'	-4.03	104.44	110.43
2	C	459	CBI	O4-C4-C3	-4.00	101.33	110.34
2	A	459	CBI	O5-C1-C2	-3.97	102.13	110.28
2	A	460	CBI	O2-C2-C3	-3.95	101.45	110.34
2	A	459	CBI	O4'-C4'-C5'	-3.91	99.04	109.32
2	C	459	CBI	O4'-C1-O5	-3.45	101.95	110.68
2	A	459	CBI	C1'-C2'-C3'	-3.42	105.35	110.43
2	B	460	CBI	O4'-C4'-C3'	-3.38	98.43	107.17
2	A	459	CBI	O4-C4-C5	-3.38	100.29	109.24
2	A	459	CBI	C3-C4-C5	-3.22	104.59	110.20
2	C	459	CBI	C3'-C4'-C5'	-3.20	103.61	110.84
2	C	459	CBI	O2-C2-C3	-3.18	103.18	110.34
2	A	459	CBI	C1-C2-C3	-3.11	103.85	109.97
2	A	460	CBI	O1'-C1'-O5'	-3.04	101.94	110.25
2	B	460	CBI	C1-C2-C3	-3.02	104.03	109.97
2	B	459	CBI	O2'-C2'-C1'	-3.01	103.18	109.21
2	B	460	CBI	O2-C2-C3	-2.99	103.61	110.34
2	A	459	CBI	O6-C6-C5	-2.97	101.53	111.33
2	B	459	CBI	C3-C4-C5	-2.71	105.47	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	459	CBI	C1-O5-C5	-2.45	108.99	113.75
2	C	459	CBI	O4'-C4'-C3'	-2.44	100.86	107.17
2	B	459	CBI	O2-C2-C1	-2.36	104.85	110.02
2	B	460	CBI	O2'-C2'-C3'	-2.34	105.06	110.34
2	B	460	CBI	O4-C4-C5	-2.33	103.06	109.24
2	A	460	CBI	C1-O4'-C4'	-2.32	111.94	118.01
2	A	460	CBI	O2-C2-C1	-2.31	104.95	110.02
2	B	459	CBI	O3'-C3'-C2'	-2.28	105.88	110.00
2	C	459	CBI	C1-C2-C3	-2.26	105.52	109.97
2	B	460	CBI	C1'-C2'-C3'	-2.23	107.11	110.43
2	C	460	CBI	O2'-C2'-C3'	-2.11	105.59	110.34
2	A	460	CBI	C1-C2-C3	-2.07	105.89	109.97
2	B	460	CBI	O5-C1-C2	-2.05	106.06	110.28
2	C	459	CBI	O2'-C2'-C1'	-2.05	105.09	109.21
2	A	459	CBI	O2'-C2'-C3'	-2.00	105.83	110.34
2	A	460	CBI	O3-C3-C2	2.03	114.90	110.34
2	C	460	CBI	O3-C3-C2	2.05	114.95	110.34
2	B	460	CBI	O1'-C1'-O5'	2.05	115.85	110.25
2	C	460	CBI	C4-C3-C2	2.08	114.68	110.79
2	A	459	CBI	O4'-C1-C2	2.11	113.23	108.10
2	C	460	CBI	O1'-C1'-C2'	2.19	115.08	109.21
2	C	459	CBI	O3-C3-C2	2.33	115.57	110.34
2	B	459	CBI	O5'-C5'-C4'	2.39	114.36	110.01
2	C	460	CBI	O3-C3-C4	2.39	115.73	110.34
2	A	460	CBI	O3'-C3'-C2'	2.40	115.73	110.34
2	C	459	CBI	C6'-C5'-C4'	2.44	120.34	113.25
2	B	460	CBI	O1'-C1'-C2'	2.51	115.95	109.21
2	C	460	CBI	C2'-C3'-C4'	2.67	115.47	109.60
2	C	459	CBI	O3-C3-C4	2.72	116.47	110.34
2	A	459	CBI	O3'-C3'-C4'	2.75	116.38	109.87
2	B	459	CBI	O3-C3-C2	2.80	116.63	110.34
2	A	460	CBI	O5-C5-C6	2.85	113.56	106.36
2	B	460	CBI	C1-O4'-C4'	2.86	125.47	118.01
2	C	459	CBI	O5'-C5'-C4'	2.88	115.26	110.01
2	C	460	CBI	O6'-C6'-C5'	2.89	120.87	111.33
2	B	459	CBI	O5-C5-C4	2.90	115.13	109.68
2	A	459	CBI	C4-C3-C2	2.97	116.33	110.79
2	A	460	CBI	O3'-C3'-C4'	3.01	116.99	109.87
2	C	459	CBI	O4'-C1-C2	3.12	115.70	108.10
2	A	460	CBI	O5-C5-C4	3.18	115.64	109.68
2	B	460	CBI	O3-C3-C2	3.22	117.59	110.34
2	A	460	CBI	C4-C3-C2	3.24	116.84	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	460	CBI	O5-C1-C2	3.28	117.00	110.28
2	A	459	CBI	C2'-C3'-C4'	3.29	116.83	109.60
2	A	459	CBI	O5'-C1'-C2'	3.34	115.12	109.80
2	C	460	CBI	O5'-C5'-C6'	3.53	115.28	106.36
2	C	459	CBI	O5-C5-C6	3.76	115.86	106.36
2	A	460	CBI	O5'-C5'-C4'	3.79	117.75	109.75
2	C	460	CBI	O3'-C3'-C4'	3.80	118.86	109.87
2	A	460	CBI	O3-C3-C4	3.85	118.99	110.34
2	A	460	CBI	O5'-C1'-C2'	3.88	115.99	109.80
2	B	459	CBI	C1-O5-C5	3.99	121.50	113.75
2	C	460	CBI	C6'-C5'-C4'	4.00	124.89	113.25
2	A	460	CBI	O5'-C5'-C6'	4.09	116.69	106.36
2	B	460	CBI	O4'-C1-O5	4.17	121.23	110.68
2	C	460	CBI	C6-C5-C4	4.20	123.38	113.02
2	A	459	CBI	C1-O4'-C4'	4.29	129.22	118.01
2	B	459	CBI	C6'-C5'-C4'	4.33	125.85	113.25
2	A	459	CBI	O5-C5-C6	4.51	117.76	106.36
2	B	460	CBI	O3-C3-C4	5.15	121.94	110.34
2	B	459	CBI	O5'-C5'-C6'	5.16	118.52	107.35
2	A	460	CBI	C1'-O5'-C5'	5.29	123.25	113.47
2	A	459	CBI	C1'-O5'-C5'	5.46	123.56	113.47
2	C	460	CBI	O5-C5-C6	5.50	120.25	106.36
2	A	459	CBI	C6-C5-C4	6.41	128.84	113.02
2	C	459	CBI	O5'-C5'-C6'	7.64	123.90	107.35
2	B	459	CBI	O4'-C1-C2	7.85	127.19	108.10
2	B	459	CBI	C1'-O5'-C5'	7.96	122.35	112.25
2	B	459	CBI	O5-C5-C6	8.01	126.60	106.36
2	C	459	CBI	C1'-O5'-C5'	8.64	123.21	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	459	CBI	C5'
2	B	459	CBI	C5'
2	B	459	CBI	C5
2	A	459	CBI	C5

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	459	CBI	2	0
2	C	459	CBI	3	0
2	C	460	CBI	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	377/458 (82%)	0.06	18 (4%)	34	36	16, 30, 50, 59	11 (2%)
1	B	379/458 (82%)	0.09	17 (4%)	37	38	16, 33, 57, 68	10 (2%)
1	C	378/458 (82%)	0.27	13 (3%)	49	50	22, 44, 63, 80	9 (2%)
All	All	1134/1374 (82%)	0.14	48 (4%)	40	41	16, 34, 59, 80	30 (2%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	TYR	9.1
1	B	33	TYR	5.8
1	B	44	ARG	5.3
1	B	32	THR	4.8
1	C	136	MET	4.3
1	A	311	PRO	4.3
1	A	136	MET	4.0
1	B	286	ASN	3.9
1	A	223	GLY	3.7
1	C	286	ASN	3.7
1	B	311	PRO	3.7
1	C	161	HIS	3.7
1	B	312	ALA	3.7
1	A	221	GLY	3.6
1	C	314	GLY	3.4
1	B	122	SER	3.4
1	A	167	TYR	3.3
1	B	128	ARG	3.2
1	A	312	ALA	3.1
1	A	310	GLY	3.1
1	C	34	GLN	3.1
1	A	259	PRO	3.0
1	A	368	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	174	GLU	3.0
1	A	286	ASN	3.0
1	C	315	PHE	3.0
1	A	161	HIS	2.9
1	B	121	TYR	2.9
1	B	130	LEU	2.8
1	B	234	GLU	2.8
1	B	82	TRP	2.8
1	B	368	GLU	2.6
1	A	282	ASP	2.6
1	A	234	GLU	2.5
1	A	263	SER	2.5
1	A	108	GLU	2.5
1	C	171	PHE	2.4
1	B	310	GLY	2.4
1	C	242	LYS	2.3
1	A	283	TYR	2.3
1	C	336	TYR	2.3
1	A	260	LYS	2.3
1	A	264	SER	2.2
1	B	113	GLY	2.1
1	C	53	VAL	2.1
1	B	91	LEU	2.1
1	C	319	LEU	2.1
1	C	170	ASP	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	CBI	A	459	23/23	0.58	0.31	14.05	40,47,49,50	0
2	CBI	C	459	22/23	0.56	0.29	12.90	50,62,69,70	0
2	CBI	B	459	22/23	0.50	0.29	11.30	53,56,58,59	0
2	CBI	B	460	23/23	0.91	0.15	2.57	31,40,44,48	0
3	PO4	A	463	5/5	0.95	0.14	1.19	54,54,56,56	0
2	CBI	A	460	23/23	0.81	0.16	1.00	44,50,54,57	0
2	CBI	C	460	23/23	0.86	0.12	0.06	48,53,56,58	0
3	PO4	A	461	5/5	0.97	0.11	-1.27	36,37,39,40	0
3	PO4	A	462	5/5	0.98	0.07	-2.89	43,43,45,46	0

6.5 Other polymers (i)

There are no such residues in this entry.