Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:36 PM GMT

PDB ID	:	4FIQ
Title	:	Crystal structure of pyridoxal biosynthesis lyase PdxS from Pyrococcus horikoshii
Authors	:	Matsuura, A.; Yoon, J.Y.; Yoon, H.J.; Lee, H.H.; Suh, S.W.
Deposited on	:	2012-06-11
Resolution	:	2.70 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:

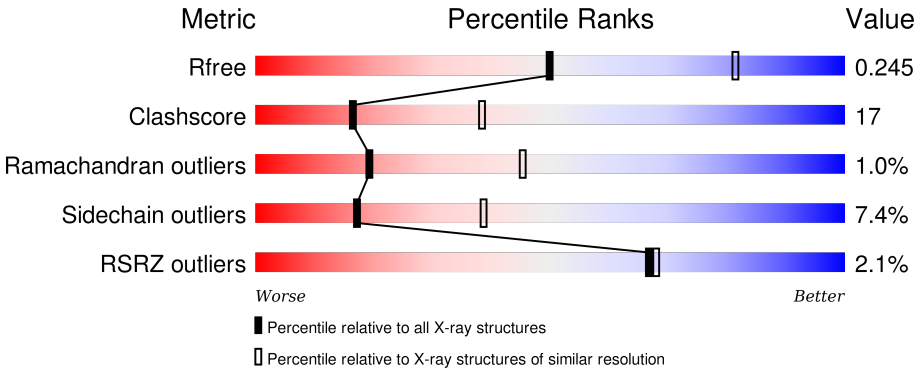
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	335	73% 19% • 6%
1	B	335	3% 59% 30% 6% • •
1	C	335	4% 65% 28% • •
1	D	335	2% 67% 27% • •
1	E	335	% 66% 27% • •

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Mol	Chain	Length	Quality of chain
1	F	335	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15128 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 Pyridoxal biosynthesis lyase pdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2424	1543	424	440	17			
1	B	321	Total	C	N	O	S	0	0	0
			2472	1571	434	449	18			
1	C	321	Total	C	N	O	S	0	0	0
			2472	1571	434	449	18			
1	D	321	Total	C	N	O	S	0	0	0
			2472	1571	434	449	18			
1	E	321	Total	C	N	O	S	0	0	0
			2472	1571	434	449	18			
1	F	321	Total	C	N	O	S	0	0	0
			2472	1571	434	449	18			

- Molecule 2 is water.

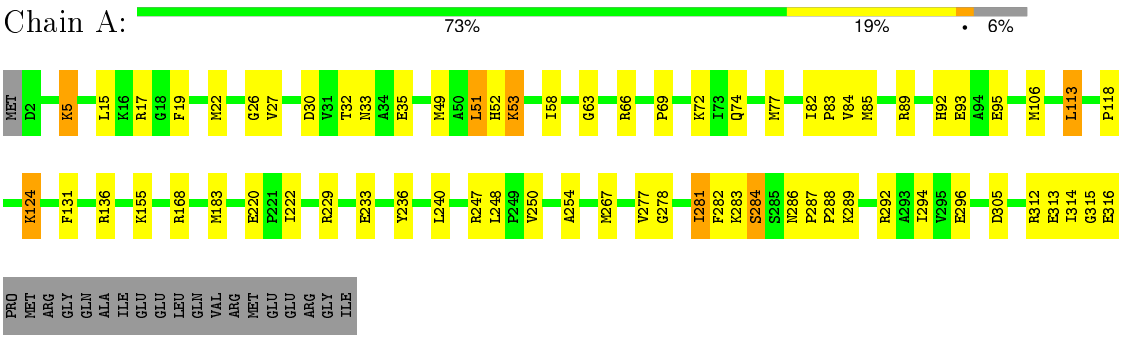
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	77	Total	O	0	0
			77	77		
2	B	52	Total	O	0	0
			52	52		
2	C	49	Total	O	0	0
			49	49		
2	D	43	Total	O	0	0
			43	43		
2	E	69	Total	O	0	0
			69	69		
2	F	54	Total	O	0	0
			54	54		

3 Residue-property plots

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.

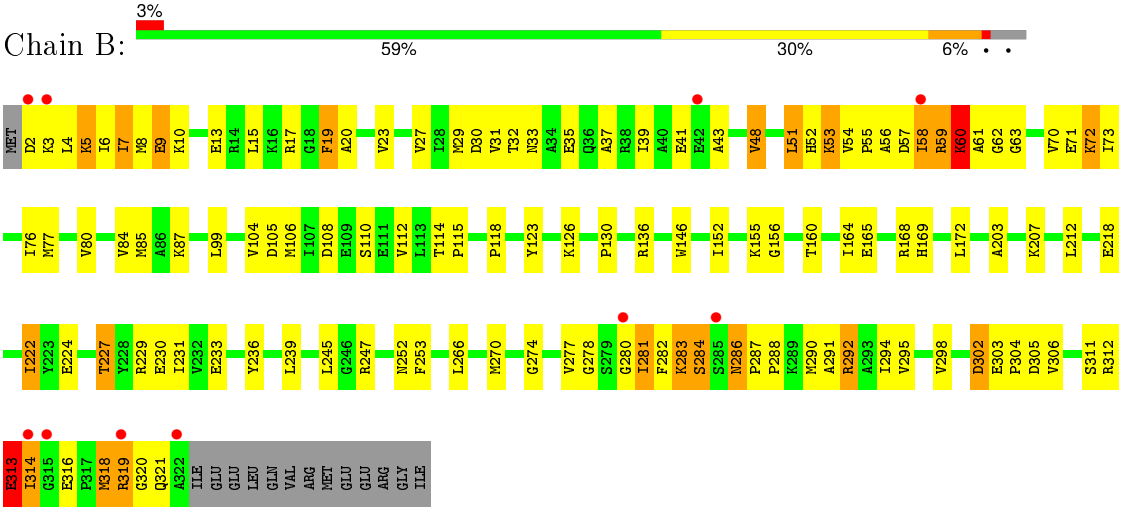
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain A:



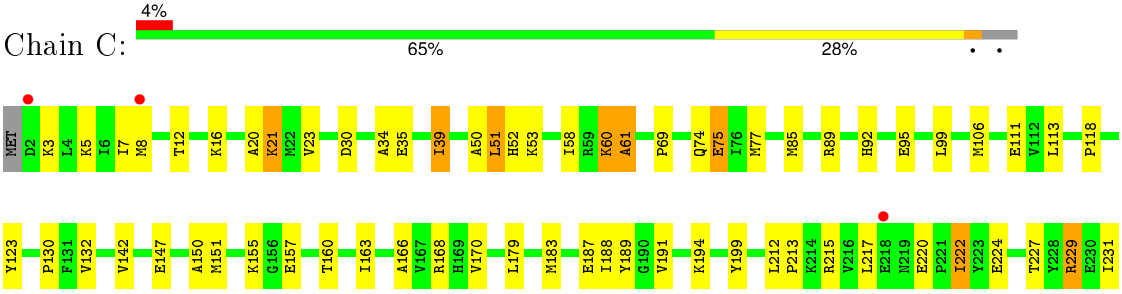
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

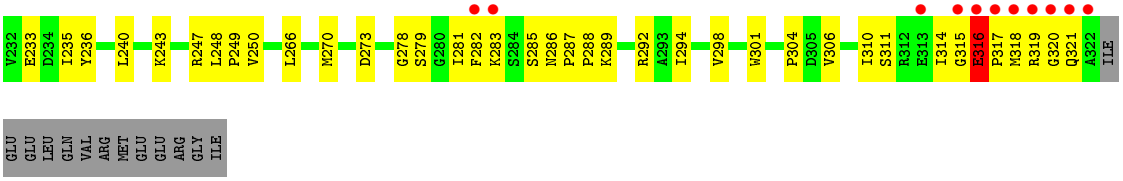
Chain B:



- Molecule 1: Pyridoxal biosynthesis lyase pdxS

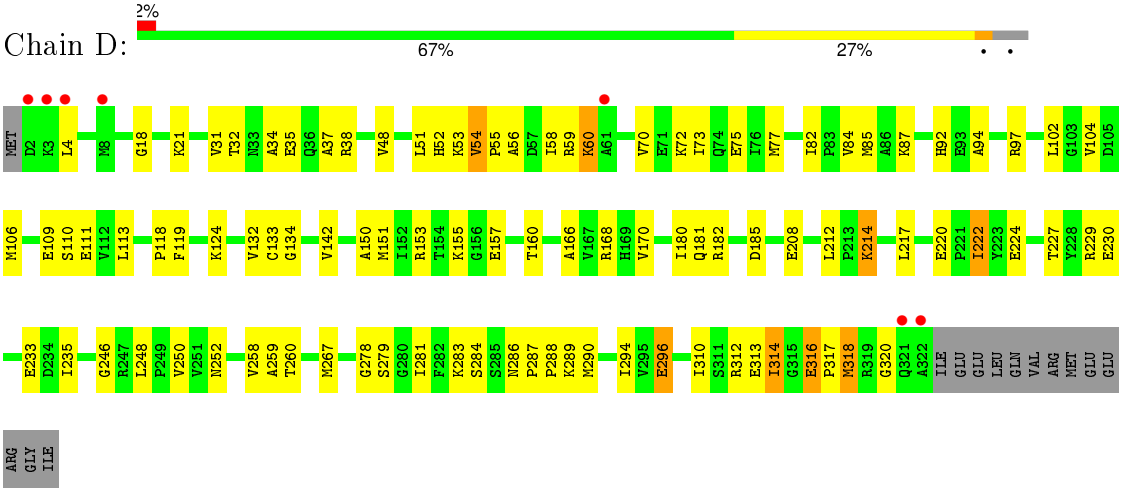
Chain C:





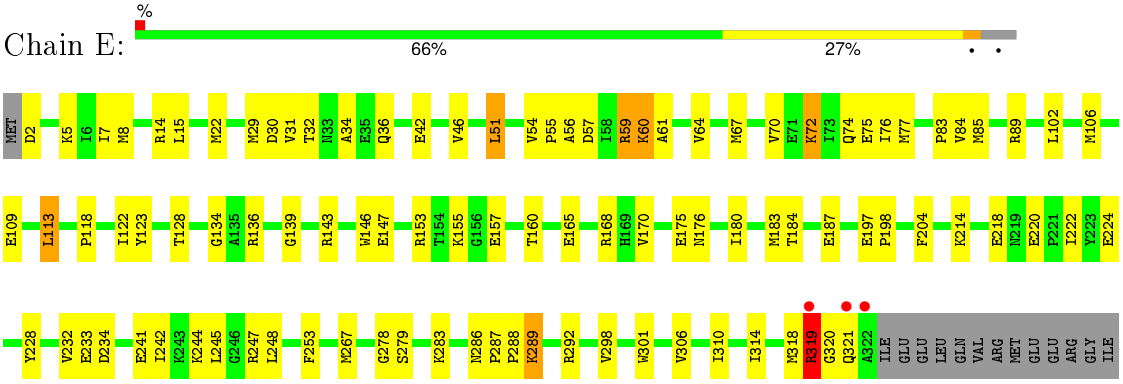
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain D:



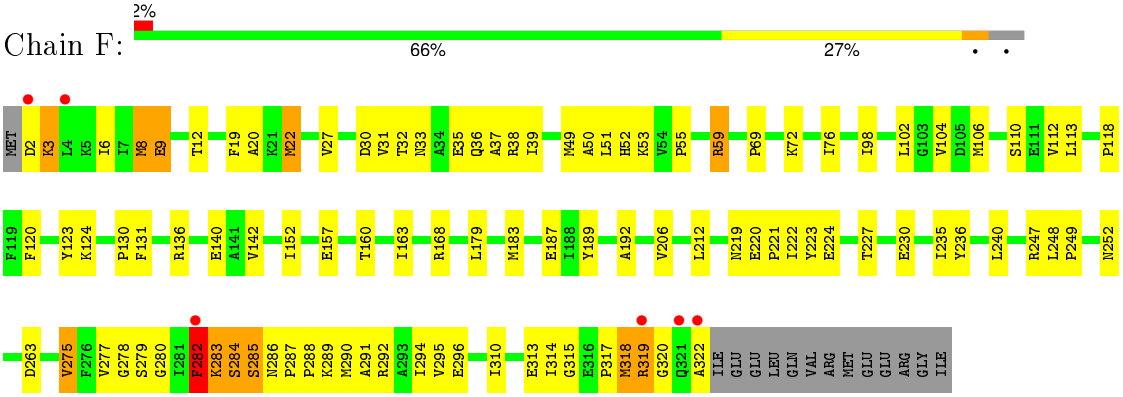
• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain E:



• Molecule 1: Pyridoxal biosynthesis lyase pdxS

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.30Å 178.56Å 109.23Å 90.00° 102.97° 90.00°	Depositor
Resolution (Å)	19.98 – 2.70 41.46 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.98-2.70) 99.5 (41.46-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.28 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.173 , 0.246 0.176 , 0.245	Depositor DCC
R_{free} test set	3093 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 66107 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15128	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

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	0.47	0/2463	0.61	0/3318
1	B	0.43	0/2512	0.57	0/3383
1	C	0.41	0/2512	0.56	0/3383
1	D	0.42	0/2512	0.56	0/3383
1	E	0.46	0/2512	0.60	1/3383 (0.0%)
1	F	0.43	0/2512	0.59	0/3383
All	All	0.44	0/15023	0.58	1/20233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	51	LEU	CA-CB-CG	6.05	129.22	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2424	0	2500	67	0
1	B	2472	0	2549	113	0
1	C	2472	0	2549	82	0
1	D	2472	0	2549	78	0
1	E	2472	0	2549	73	0
1	F	2472	0	2549	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	77	0	0	5	0
2	B	52	0	0	0	0
2	C	49	0	0	2	0
2	D	43	0	0	2	0
2	E	69	0	0	2	0
2	F	54	0	0	1	0
All	All	15128	0	15245	499	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 17.

All (499) 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:F:319:ARG:HH11	1:F:319:ARG:HG2	1.13	1.10
1:F:59:ARG:HG3	1:F:59:ARG:HH11	1.09	1.08
1:A:53:LYS:HD3	1:A:53:LYS:H	1.22	1.02
1:B:60:LYS:H	1:B:60:LYS:HZ1	0.99	0.96
1:B:60:LYS:HZ2	1:B:60:LYS:HB2	1.28	0.96
1:B:227:THR:HG22	1:B:230:GLU:H	1.32	0.94
1:B:59:ARG:HG2	1:B:60:LYS:HE3	1.51	0.92
1:C:52:HIS:CD2	1:C:53:LYS:HG3	2.05	0.92
1:B:60:LYS:NZ	1:B:60:LYS:H	1.67	0.91
1:C:168:ARG:HB2	1:D:118:PRO:HG3	1.53	0.90
1:A:53:LYS:HG2	1:A:58:ILE:HD11	1.54	0.90
1:B:247:ARG:HG3	1:B:247:ARG:HH11	1.37	0.89
1:F:59:ARG:HG3	1:F:59:ARG:NH1	1.86	0.89
1:E:56:ALA:HA	1:E:59:ARG:HB2	1.53	0.88
1:F:319:ARG:HG2	1:F:319:ARG:NH1	1.85	0.88
1:D:260:THR:HA	1:D:290:MET:HE1	1.54	0.87
1:E:2:ASP:HB3	1:E:5:LYS:HG2	1.55	0.87
1:B:283:LYS:O	1:B:287:PRO:HG3	1.74	0.87
1:C:316:GLU:CG	1:C:317:PRO:HA	2.05	0.87
1:A:53:LYS:CD	1:A:53:LYS:H	1.88	0.86
1:D:181:GLN:NE2	1:D:246:GLY:HA2	1.90	0.86
1:B:59:ARG:HB2	1:B:63:GLY:O	1.76	0.85
1:F:52:HIS:CG	1:F:53:LYS:H	1.93	0.85
1:E:136:ARG:HG3	1:E:155:LYS:HD2	1.57	0.85
1:C:316:GLU:HG3	1:C:317:PRO:HA	1.57	0.84
1:B:60:LYS:N	1:B:60:LYS:HZ1	1.76	0.83
1:B:58:ILE:HG12	1:B:61:ALA:HB3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:HIS:CD2	1:F:53:LYS:H	1.98	0.82
1:A:53:LYS:N	1:A:53:LYS:CD	2.45	0.80
1:B:284:SER:HB2	1:B:316:GLU:H	1.46	0.80
1:B:283:LYS:HD2	1:B:318:MET:HB3	1.63	0.80
1:E:29:MET:HB3	2:E:443:HOH:O	1.83	0.79
1:E:60:LYS:HG3	1:E:61:ALA:H	1.47	0.78
1:B:30:ASP:HB2	1:B:278:GLY:HA2	1.65	0.78
1:C:85:MET:HG2	1:C:106:MET:HB3	1.65	0.77
1:A:53:LYS:N	1:A:53:LYS:HD3	2.00	0.77
1:C:316:GLU:CB	1:C:317:PRO:HA	2.16	0.76
1:D:56:ALA:HB1	1:D:60:LYS:NZ	1.99	0.76
1:F:9:GLU:HA	1:F:12:THR:HB	1.67	0.76
1:E:54:VAL:O	1:E:57:ASP:HB2	1.86	0.76
1:F:291:ALA:O	1:F:295:VAL:HG23	1.85	0.76
1:E:85:MET:HG2	1:E:106:MET:HB3	1.69	0.75
1:F:142:VAL:HG11	1:F:235:ILE:HG23	1.69	0.75
1:F:286:ASN:ND2	1:F:289:LYS:HD2	2.00	0.75
1:F:52:HIS:CG	1:F:53:LYS:N	2.52	0.74
1:D:18:GLY:HA2	1:D:21:LYS:HD3	1.69	0.74
1:D:73:ILE:O	1:D:77:MET:HG3	1.87	0.74
1:F:285:SER:O	1:F:287:PRO:HD3	1.88	0.74
1:B:110:SER:OG	1:B:112:VAL:HG22	1.87	0.74
1:E:319:ARG:CB	1:E:320:GLY:HA2	2.18	0.74
1:E:286:ASN:ND2	1:E:289:LYS:HB2	2.02	0.74
1:F:313:GLU:O	1:F:314:ILE:HG13	1.88	0.73
1:A:19:PHE:O	1:A:22:MET:HG2	1.87	0.73
1:C:316:GLU:HG3	1:C:317:PRO:CA	2.20	0.72
1:F:285:SER:H	1:F:315:GLY:HA3	1.55	0.72
1:B:136:ARG:HG3	1:B:155:LYS:HD2	1.70	0.72
1:F:313:GLU:C	1:F:314:ILE:HG13	2.10	0.72
1:F:2:ASP:O	1:F:6:ILE:HG12	1.90	0.72
1:E:319:ARG:HB2	1:E:320:GLY:HA2	1.71	0.71
1:D:227:THR:HG21	2:D:434:HOH:O	1.89	0.71
1:F:31:VAL:HG11	1:F:37:ALA:HA	1.72	0.71
1:F:123:TYR:CD2	1:F:224:GLU:HG2	2.26	0.71
1:D:312:ARG:HH21	1:E:74:GLN:HG2	1.55	0.71
1:E:57:ASP:HA	1:E:60:LYS:HG2	1.73	0.70
1:A:72:LYS:HD3	1:A:72:LYS:O	1.91	0.70
1:C:287:PRO:HB2	1:C:288:PRO:HD3	1.74	0.70
1:F:183:MET:CE	1:F:187:GLU:HB3	2.22	0.69
1:B:55:PRO:O	1:B:60:LYS:NZ	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:HIS:CG	1:B:53:LYS:H	2.11	0.69
1:D:296:GLU:HB3	1:D:310:ILE:HD13	1.74	0.68
1:A:314:ILE:HG23	1:A:316:GLU:H	1.59	0.68
1:D:227:THR:CG2	1:D:230:GLU:H	2.07	0.68
1:D:51:LEU:HD11	1:D:87:LYS:HD2	1.76	0.68
1:A:283:LYS:O	1:A:284:SER:HB3	1.93	0.68
1:F:52:HIS:HB3	1:F:69:PRO:HD2	1.76	0.68
1:B:20:ALA:O	1:B:23:VAL:HG22	1.94	0.68
1:F:319:ARG:H	1:F:319:ARG:HD2	1.58	0.68
1:B:60:LYS:NZ	1:B:60:LYS:HB2	2.08	0.68
1:D:124:LYS:HE2	1:D:133:CYS:SG	2.33	0.68
1:C:316:GLU:HB3	1:C:317:PRO:HA	1.76	0.67
1:A:283:LYS:O	1:A:284:SER:CB	2.41	0.67
1:D:181:GLN:HE22	1:D:246:GLY:HA2	1.60	0.67
1:F:160:THR:O	1:F:320:GLY:HA2	1.96	0.66
1:B:59:ARG:CG	1:B:60:LYS:HE3	2.25	0.66
1:B:85:MET:HG2	1:B:106:MET:HB3	1.76	0.66
1:F:189:TYR:HA	1:F:236:TYR:HD1	1.61	0.66
1:A:288:PRO:O	1:A:289:LYS:HB3	1.95	0.66
1:B:52:HIS:CG	1:B:53:LYS:N	2.64	0.65
1:D:157:GLU:HG3	1:D:160:THR:OG1	1.95	0.65
1:F:106:MET:HB2	1:F:130:PRO:HG2	1.78	0.65
1:C:319:ARG:HH11	1:C:319:ARG:HG3	1.60	0.65
1:A:247:ARG:HG3	1:A:248:LEU:O	1.96	0.65
1:E:287:PRO:HB2	1:E:288:PRO:HD3	1.79	0.65
1:A:85:MET:HG2	1:A:106:MET:HB3	1.78	0.64
1:B:5:LYS:O	1:B:9:GLU:HB3	1.97	0.64
1:B:58:ILE:CG1	1:B:61:ALA:HB3	2.26	0.63
1:D:70:VAL:HG13	1:D:102:LEU:HD21	1.80	0.63
1:B:35:GLU:O	1:B:39:ILE:HD12	1.98	0.63
1:F:30:ASP:OD1	1:F:49:MET:HB3	1.99	0.63
1:B:5:LYS:HB3	1:B:5:LYS:NZ	2.14	0.63
1:D:150:ALA:O	1:D:250:VAL:HB	1.97	0.63
1:B:59:ARG:HG2	1:B:60:LYS:CE	2.27	0.63
1:B:283:LYS:CD	1:B:318:MET:HB3	2.28	0.63
1:C:160:THR:O	1:C:320:GLY:HA3	1.98	0.62
1:C:52:HIS:HB3	1:C:69:PRO:HD2	1.82	0.62
1:E:60:LYS:HG3	1:E:61:ALA:N	2.15	0.62
1:B:33:ASN:OD1	1:B:35:GLU:HB3	2.00	0.62
1:D:106:MET:CE	1:D:151:MET:HG2	2.30	0.62
1:B:218:GLU:OE1	1:B:229:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:O	1:B:270:MET:HG3	1.99	0.62
1:F:32:THR:HA	1:F:51:LEU:O	1.99	0.61
1:B:99:LEU:O	1:B:104:VAL:HG22	1.99	0.61
1:E:143:ARG:O	1:E:147:GLU:HG3	2.00	0.61
1:B:59:ARG:HD2	1:B:114:THR:OG1	2.01	0.61
1:D:56:ALA:HB1	1:D:60:LYS:HZ3	1.65	0.61
1:A:314:ILE:HG23	1:A:315:GLY:N	2.16	0.61
1:A:63:GLY:O	1:F:322:ALA:HB2	2.00	0.60
1:B:60:LYS:CB	1:B:60:LYS:HZ2	2.08	0.60
1:E:318:MET:HA	1:E:319:ARG:NH1	2.15	0.60
1:C:247:ARG:HG2	1:C:248:LEU:N	2.16	0.60
1:F:290:MET:CE	1:F:294:ILE:HD11	2.31	0.60
1:F:284:SER:H	1:F:285:SER:HA	1.66	0.60
1:B:58:ILE:CD1	1:B:61:ALA:HB3	2.32	0.59
1:C:316:GLU:HG3	1:C:317:PRO:C	2.23	0.59
1:F:290:MET:SD	1:F:314:ILE:HG21	2.42	0.59
1:B:59:ARG:HB2	1:B:63:GLY:C	2.22	0.59
1:E:70:VAL:HG13	1:E:102:LEU:HD21	1.84	0.59
1:A:32:THR:HG22	1:A:51:LEU:HD23	1.83	0.59
1:D:160:THR:O	1:D:320:GLY:HA2	2.02	0.59
1:B:60:LYS:NZ	1:B:60:LYS:N	2.43	0.59
1:B:227:THR:HG22	1:B:230:GLU:HG3	1.85	0.59
1:F:314:ILE:HG22	1:F:315:GLY:H	1.67	0.59
1:B:247:ARG:HG3	1:B:247:ARG:NH1	2.10	0.59
1:D:290:MET:HE3	1:D:294:ILE:HD11	1.83	0.59
1:E:183:MET:HE1	1:F:212:LEU:HD11	1.85	0.59
1:B:160:THR:HG22	1:B:321:GLN:HB2	1.85	0.59
1:F:160:THR:O	1:F:320:GLY:CA	2.51	0.58
1:E:77:MET:HA	1:E:84:VAL:HG21	1.85	0.58
1:E:30:ASP:HB2	1:E:278:GLY:HA2	1.85	0.58
1:E:55:PRO:C	1:E:57:ASP:H	2.07	0.58
1:F:179:LEU:O	1:F:183:MET:HG3	2.02	0.58
1:A:5:LYS:NZ	1:A:5:LYS:HB3	2.18	0.58
1:C:20:ALA:O	1:C:23:VAL:HG22	2.03	0.58
1:C:89:ARG:HG2	1:C:113:LEU:HB3	1.85	0.58
1:B:19:PHE:CD2	1:B:19:PHE:C	2.76	0.58
1:F:284:SER:N	1:F:285:SER:HA	2.19	0.58
1:E:2:ASP:CB	1:E:5:LYS:HG2	2.29	0.58
1:F:30:ASP:HB2	1:F:278:GLY:HA2	1.85	0.57
1:C:85:MET:HE1	1:C:106:MET:SD	2.45	0.57
1:A:17:ARG:HD3	1:A:250:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:MET:HE1	1:F:187:GLU:HB3	1.87	0.57
1:B:19:PHE:CZ	1:B:105:ASP:HB3	2.39	0.57
1:D:111:GLU:HG3	1:D:155:LYS:HD3	1.86	0.57
1:E:157:GLU:HG3	1:E:160:THR:HG21	1.87	0.56
1:B:286:ASN:N	1:B:287:PRO:HD3	2.20	0.56
1:B:30:ASP:HB2	1:B:278:GLY:CA	2.33	0.56
1:A:89:ARG:HG2	1:A:113:LEU:HB3	1.86	0.56
1:B:302:ASP:O	1:B:304:PRO:HD3	2.05	0.56
1:F:189:TYR:HA	1:F:236:TYR:CD1	2.41	0.56
1:B:77:MET:HE3	1:B:104:VAL:HA	1.87	0.56
1:E:31:VAL:HG23	1:E:76:ILE:HD13	1.87	0.56
1:E:57:ASP:O	1:E:60:LYS:HG3	2.05	0.56
1:E:306:VAL:HG12	1:E:310:ILE:CD1	2.36	0.56
1:F:319:ARG:H	1:F:319:ARG:CD	2.16	0.56
1:D:227:THR:HG23	1:D:229:ARG:N	2.21	0.56
1:B:19:PHE:HZ	1:B:105:ASP:HB3	1.71	0.55
1:D:289:LYS:HD3	1:D:314:ILE:HD12	1.88	0.55
1:B:203:ALA:O	1:B:207:LYS:HG2	2.06	0.55
1:D:106:MET:HE2	1:D:151:MET:HG2	1.87	0.55
1:C:247:ARG:NH2	1:C:273:ASP:OD1	2.39	0.55
1:F:9:GLU:CD	1:F:9:GLU:H	2.10	0.55
1:B:87:LYS:HG2	1:B:108:ASP:HB3	1.89	0.55
1:B:291:ALA:O	1:B:295:VAL:HG23	2.07	0.55
1:B:19:PHE:HD2	1:B:19:PHE:C	2.09	0.55
1:E:180:ILE:O	1:E:183:MET:HB2	2.06	0.54
1:B:168:ARG:HG2	1:B:172:LEU:HD12	1.90	0.54
1:D:227:THR:HG22	1:D:230:GLU:H	1.71	0.54
1:B:227:THR:CG2	1:B:230:GLU:H	2.13	0.54
1:B:156:GLY:H	1:B:169:HIS:CE1	2.25	0.54
1:E:2:ASP:HB3	1:E:5:LYS:CG	2.33	0.53
1:C:60:LYS:O	1:C:61:ALA:HB2	2.08	0.53
1:F:290:MET:HE1	1:F:294:ILE:HD11	1.90	0.53
1:F:314:ILE:HG22	1:F:315:GLY:N	2.22	0.53
1:D:142:VAL:HG11	1:D:235:ILE:HG23	1.91	0.53
1:A:312:ARG:HG2	1:A:312:ARG:O	2.08	0.53
1:C:229:ARG:O	1:C:233:GLU:HG2	2.07	0.53
1:E:55:PRO:O	1:E:56:ALA:HB3	2.08	0.53
1:E:168:ARG:HB2	1:F:118:PRO:HG3	1.90	0.53
1:F:313:GLU:O	1:F:314:ILE:CG1	2.55	0.53
1:B:282:PHE:O	1:B:283:LYS:HG3	2.08	0.53
1:E:89:ARG:HG2	1:E:113:LEU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:HD13	1:B:314:ILE:H	1.74	0.53
1:A:32:THR:HG22	1:A:51:LEU:CD2	2.39	0.53
1:F:220:GLU:O	1:F:222:ILE:HG12	2.07	0.53
1:D:284:SER:O	1:D:287:PRO:HD3	2.08	0.53
1:C:30:ASP:HB2	1:C:278:GLY:HA2	1.90	0.53
1:D:227:THR:HG23	1:D:230:GLU:H	1.74	0.52
1:D:217:LEU:HB2	1:D:220:GLU:OE2	2.09	0.52
1:A:136:ARG:HG3	1:A:155:LYS:HD2	1.91	0.52
1:B:60:LYS:CB	1:B:60:LYS:NZ	2.71	0.52
1:B:168:ARG:HB2	1:C:118:PRO:HG3	1.90	0.52
1:A:281:ILE:HG22	1:A:282:PHE:CD2	2.44	0.52
1:D:77:MET:HA	1:D:84:VAL:HG21	1.90	0.52
1:C:150:ALA:O	1:C:250:VAL:HB	2.10	0.52
1:A:118:PRO:HG3	1:F:168:ARG:HB2	1.92	0.52
1:C:163:ILE:HG13	1:C:163:ILE:O	2.08	0.52
1:A:296:GLU:HA	1:A:296:GLU:OE2	2.10	0.52
1:D:56:ALA:O	1:D:60:LYS:HE2	2.09	0.52
1:F:183:MET:HE2	1:F:187:GLU:HB3	1.90	0.52
1:D:56:ALA:HB1	1:D:60:LYS:HZ1	1.73	0.52
1:C:286:ASN:ND2	1:C:289:LYS:HD2	2.25	0.52
1:C:3:LYS:O	1:C:7:ILE:HG12	2.10	0.52
1:C:132:VAL:HB	1:C:151:MET:HE3	1.91	0.52
1:B:6:ILE:O	1:B:10:LYS:HB2	2.09	0.52
1:B:31:VAL:HG23	1:B:76:ILE:HD13	1.91	0.52
1:C:53:LYS:HE3	1:C:58:ILE:HD11	1.91	0.52
1:F:59:ARG:CG	1:F:59:ARG:HH11	1.99	0.51
1:A:236:TYR:CE2	1:A:240:LEU:HD11	2.45	0.51
1:C:311:SER:O	1:C:314:ILE:HD13	2.10	0.51
1:D:170:VAL:HG21	1:D:267:MET:CE	2.39	0.51
1:C:106:MET:SD	1:C:151:MET:CE	2.99	0.51
1:E:157:GLU:HG3	1:E:160:THR:CG2	2.39	0.51
1:F:285:SER:N	1:F:315:GLY:HA3	2.23	0.51
1:E:306:VAL:HG12	1:E:310:ILE:HD12	1.93	0.51
1:B:160:THR:O	1:B:320:GLY:HA3	2.11	0.51
1:B:6:ILE:HG23	1:B:7:ILE:H	1.75	0.51
1:E:109:GLU:OE2	1:E:122:ILE:HG13	2.11	0.51
1:F:36:GLN:NE2	1:F:282:PHE:CE1	2.79	0.51
1:B:6:ILE:HG23	1:B:7:ILE:N	2.25	0.51
1:D:92:HIS:CE1	1:D:94:ALA:HB3	2.46	0.51
1:F:35:GLU:O	1:F:39:ILE:HG13	2.11	0.50
1:F:319:ARG:HH11	1:F:319:ARG:CG	2.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:HG3	1:B:10:LYS:N	2.26	0.50
1:F:19:PHE:O	1:F:22:MET:HB2	2.11	0.50
1:E:241:GLU:O	1:E:245:LEU:HD12	2.11	0.50
1:B:59:ARG:O	1:B:61:ALA:N	2.44	0.50
1:B:281:ILE:HG13	1:B:282:PHE:H	1.77	0.50
1:D:92:HIS:HE1	1:D:94:ALA:HB3	1.77	0.49
1:B:43:ALA:O	1:B:292:ARG:NH1	2.44	0.49
1:F:142:VAL:CG1	1:F:235:ILE:HG23	2.41	0.49
1:C:92:HIS:CD2	1:C:95:GLU:HG3	2.48	0.49
1:B:58:ILE:HA	1:B:59:ARG:C	2.32	0.49
1:C:286:ASN:HD22	1:C:289:LYS:HD2	1.77	0.49
1:D:170:VAL:HG21	1:D:267:MET:HE1	1.94	0.49
1:C:266:LEU:O	1:C:270:MET:HG3	2.13	0.49
1:D:181:GLN:HE22	1:D:246:GLY:CA	2.24	0.49
1:F:152:ILE:O	1:F:252:ASN:HA	2.12	0.49
1:F:157:GLU:HG2	1:F:160:THR:CG2	2.43	0.49
1:B:287:PRO:N	1:B:288:PRO:HD2	2.28	0.49
1:A:220:GLU:O	1:A:222:ILE:HD13	2.13	0.49
1:A:30:ASP:OD1	1:A:49:MET:HB3	2.13	0.49
1:F:319:ARG:NH1	1:F:319:ARG:CG	2.65	0.49
1:F:286:ASN:HD22	1:F:289:LYS:HD2	1.77	0.49
1:C:95:GLU:O	1:C:99:LEU:HG	2.13	0.49
1:F:247:ARG:HG3	1:F:247:ARG:HH11	1.78	0.49
1:A:314:ILE:HG23	1:A:315:GLY:H	1.77	0.49
1:F:296:GLU:OE1	1:F:296:GLU:HA	2.13	0.49
1:C:50:ALA:O	1:C:51:LEU:HD13	2.13	0.49
1:E:56:ALA:HA	1:E:59:ARG:CB	2.35	0.48
1:D:227:THR:HG22	1:D:230:GLU:CD	2.33	0.48
1:B:4:LEU:C	1:B:6:ILE:H	2.16	0.48
1:E:298:VAL:O	1:E:301:TRP:HD1	1.94	0.48
1:B:311:SER:O	1:B:314:ILE:HG23	2.13	0.48
1:A:183:MET:HE1	1:B:212:LEU:HD11	1.96	0.48
1:E:134:GLY:HA2	1:E:153:ARG:O	2.13	0.48
1:C:236:TYR:CZ	1:C:240:LEU:HD11	2.49	0.48
1:C:157:GLU:HG2	2:C:440:HOH:O	2.13	0.48
1:C:191:VAL:O	1:C:194:LYS:HB3	2.12	0.48
1:B:56:ALA:O	1:B:60:LYS:HB2	2.14	0.48
1:A:287:PRO:HA	2:A:447:HOH:O	2.12	0.48
1:E:153:ARG:HA	1:E:253:PHE:O	2.14	0.48
1:A:52:HIS:HB2	1:A:69:PRO:HD2	1.95	0.48
1:C:52:HIS:NE2	1:C:53:LYS:HG3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG11	1:B:37:ALA:HA	1.96	0.48
1:F:27:VAL:HG22	1:F:275:VAL:HG12	1.95	0.48
1:E:46:VAL:O	1:E:83:PRO:HD2	2.13	0.48
1:A:52:HIS:HB3	1:A:53:LYS:HD2	1.96	0.48
1:B:53:LYS:O	1:B:55:PRO:HD3	2.14	0.48
1:A:287:PRO:C	1:A:288:PRO:O	2.50	0.48
1:F:219:ASN:O	1:F:221:PRO:HD3	2.14	0.48
1:E:175:GLU:HG3	1:F:206:VAL:HG21	1.95	0.48
1:F:98:ILE:O	1:F:102:LEU:HB2	2.14	0.48
1:A:32:THR:O	1:A:33:ASN:HB3	2.14	0.47
1:C:60:LYS:O	1:C:60:LYS:HG3	2.14	0.47
1:D:217:LEU:HD12	1:D:220:GLU:OE2	2.14	0.47
1:D:296:GLU:HB3	1:D:310:ILE:CD1	2.44	0.47
1:D:132:VAL:HG23	1:D:151:MET:HG3	1.96	0.47
1:D:118:PRO:HG2	1:D:119:PHE:CD1	2.49	0.47
1:D:281:ILE:O	1:D:284:SER:HB3	2.13	0.47
1:F:283:LYS:O	1:F:283:LYS:HG2	2.15	0.47
1:A:52:HIS:HB3	1:A:53:LYS:CD	2.44	0.47
1:A:314:ILE:CG2	1:A:315:GLY:N	2.76	0.47
1:C:304:PRO:HB3	1:D:97:ARG:HB3	1.95	0.47
1:D:260:THR:HA	1:D:290:MET:CE	2.36	0.47
1:D:18:GLY:O	1:D:21:LYS:HB2	2.15	0.47
1:F:189:TYR:HD1	1:F:236:TYR:CD1	2.32	0.47
1:B:5:LYS:HB3	1:B:5:LYS:HZ2	1.80	0.47
1:B:4:LEU:HD13	1:B:7:ILE:HG23	1.95	0.47
1:F:283:LYS:CD	1:F:283:LYS:H	2.27	0.47
1:E:247:ARG:HG3	1:E:248:LEU:N	2.29	0.47
1:A:32:THR:O	1:A:72:LYS:NZ	2.39	0.47
1:C:217:LEU:HD12	1:C:220:GLU:OE2	2.14	0.47
1:B:105:ASP:O	1:B:130:PRO:HD2	2.15	0.47
1:B:32:THR:HA	1:B:51:LEU:O	2.15	0.47
1:D:208:GLU:HB2	1:D:214:LYS:HE2	1.96	0.47
1:B:253:PHE:CZ	1:B:274:GLY:HA3	2.49	0.47
1:B:164:ILE:HG23	1:B:165:GLU:N	2.30	0.47
1:E:55:PRO:C	1:E:57:ASP:N	2.68	0.47
1:B:146:TRP:CH2	1:B:231:ILE:HG12	2.50	0.47
1:F:290:MET:HE3	1:F:294:ILE:HD11	1.95	0.47
1:F:290:MET:HB2	1:F:314:ILE:CG2	2.45	0.47
1:A:314:ILE:CG2	1:A:315:GLY:H	2.27	0.47
1:A:284:SER:OG	2:A:447:HOH:O	2.20	0.47
1:D:53:LYS:HG3	1:D:58:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:VAL:O	1:C:310:ILE:HG13	2.14	0.47
1:E:184:THR:N	1:E:187:GLU:OE1	2.34	0.46
1:D:32:THR:O	1:D:72:LYS:HE3	2.15	0.46
1:A:53:LYS:N	1:A:53:LYS:HD2	2.27	0.46
1:D:290:MET:CE	1:D:294:ILE:HD11	2.46	0.46
1:D:283:LYS:HB2	1:D:318:MET:HE3	1.96	0.46
1:F:278:GLY:C	1:F:280:GLY:H	2.19	0.46
1:C:286:ASN:ND2	1:C:289:LYS:HB2	2.31	0.46
1:A:254:ALA:CB	1:A:267:MET:HE2	2.46	0.46
1:E:183:MET:CE	1:F:212:LEU:HD11	2.45	0.46
1:F:247:ARG:HG3	1:F:248:LEU:N	2.31	0.46
1:C:222:ILE:HD12	1:C:222:ILE:HA	1.75	0.46
1:D:259:ALA:O	1:D:290:MET:HE1	2.15	0.46
1:A:124:LYS:HG2	1:A:131:PHE:CG	2.51	0.46
1:E:204:PHE:HB3	1:E:214:LYS:HG2	1.96	0.46
1:C:227:THR:O	1:C:231:ILE:HG13	2.16	0.46
1:A:124:LYS:HG3	1:A:131:PHE:CD2	2.50	0.46
1:B:123:TYR:CD2	1:B:224:GLU:HG2	2.50	0.46
1:D:109:GLU:OE1	1:D:124:LYS:HE3	2.16	0.45
1:A:277:VAL:HG11	1:A:294:ILE:HG21	1.98	0.45
1:A:220:GLU:HG2	1:A:222:ILE:CD1	2.46	0.45
1:F:136:ARG:NH2	1:F:140:GLU:OE2	2.48	0.45
1:C:279:SER:HA	1:C:282:PHE:CD2	2.51	0.45
1:C:248:LEU:HA	1:C:249:PRO:HD3	1.82	0.45
1:B:286:ASN:N	1:B:287:PRO:CD	2.79	0.45
1:F:8:MET:HA	1:F:8:MET:CE	2.45	0.45
1:B:71:GLU:HG2	1:B:72:LYS:N	2.31	0.45
1:A:168:ARG:HB2	1:B:118:PRO:HG3	1.99	0.45
1:B:227:THR:HG23	1:B:229:ARG:H	1.81	0.45
1:D:222:ILE:HA	1:D:222:ILE:HD12	1.74	0.45
1:C:123:TYR:CD2	1:C:224:GLU:HG2	2.52	0.45
1:B:77:MET:HA	1:B:84:VAL:HG21	1.99	0.45
1:B:59:ARG:O	1:B:62:GLY:N	2.48	0.45
1:F:278:GLY:O	1:F:280:GLY:N	2.47	0.45
1:D:34:ALA:O	1:D:38:ARG:HG3	2.17	0.45
1:B:146:TRP:CZ2	1:B:231:ILE:HG12	2.52	0.45
1:B:227:THR:CG2	1:B:230:GLU:HG3	2.45	0.45
1:C:166:ALA:O	1:C:170:VAL:HG23	2.17	0.45
1:D:314:ILE:HA	1:D:314:ILE:HD12	1.81	0.45
1:C:188:ILE:HD11	1:C:243:LYS:HD2	1.99	0.45
1:F:157:GLU:CD	1:F:160:THR:HG21	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:MET:HE3	1:D:104:VAL:HA	1.99	0.44
1:C:188:ILE:CD1	1:C:243:LYS:HD2	2.47	0.44
1:A:288:PRO:O	1:A:289:LYS:CB	2.60	0.44
1:C:310:ILE:O	1:C:314:ILE:HD11	2.17	0.44
1:F:247:ARG:NH1	1:F:248:LEU:O	2.50	0.44
1:E:176:ASN:HA	1:F:206:VAL:HG11	1.99	0.44
1:B:290:MET:O	1:B:294:ILE:HG12	2.17	0.44
1:C:74:GLN:HA	1:C:77:MET:CE	2.48	0.44
1:C:298:VAL:O	1:C:301:TRP:HD1	2.00	0.44
1:B:152:ILE:O	1:B:252:ASN:HA	2.17	0.44
1:F:52:HIS:ND1	1:F:53:LYS:HG3	2.33	0.44
1:C:319:ARG:NH2	1:D:58:ILE:HD12	2.33	0.44
1:B:73:ILE:O	1:B:77:MET:HG3	2.16	0.44
1:C:111:GLU:HG3	1:C:155:LYS:HD3	1.99	0.44
1:D:31:VAL:HG11	1:D:37:ALA:HA	1.98	0.44
1:E:170:VAL:HG21	1:E:267:MET:HE1	2.00	0.44
1:A:72:LYS:C	1:A:72:LYS:HD3	2.36	0.44
1:A:77:MET:HA	1:A:84:VAL:HG21	2.00	0.44
1:C:247:ARG:HH22	1:C:273:ASP:CG	2.20	0.44
1:B:319:ARG:NE	1:B:319:ARG:H	2.16	0.44
1:E:286:ASN:HD21	1:E:289:LYS:HG3	1.82	0.44
1:A:51:LEU:HB2	2:A:439:HOH:O	2.17	0.44
1:D:320:GLY:HA3	1:E:64:VAL:HG23	2.00	0.44
1:F:227:THR:OG1	1:F:230:GLU:HG3	2.17	0.44
1:E:72:LYS:NZ	1:E:72:LYS:HB2	2.33	0.44
1:B:227:THR:HG23	1:B:229:ARG:N	2.33	0.44
1:D:56:ALA:HA	1:D:59:ARG:HD2	1.99	0.44
1:C:147:GLU:OE2	1:C:199:TYR:OH	2.32	0.44
1:E:228:TYR:O	1:E:232:VAL:HG23	2.18	0.44
1:B:303:GLU:HB3	1:B:306:VAL:HG23	1.99	0.44
1:C:53:LYS:NZ	1:C:53:LYS:HB3	2.33	0.43
1:E:54:VAL:HG12	1:E:55:PRO:O	2.18	0.43
1:D:182:ARG:CZ	1:E:220:GLU:HG3	2.48	0.43
1:E:157:GLU:HB2	1:E:165:GLU:HG3	2.00	0.43
1:C:12:THR:HG22	1:C:16:LYS:HE2	2.00	0.43
1:D:286:ASN:OD1	1:D:288:PRO:HD2	2.18	0.43
1:C:279:SER:O	1:C:282:PHE:HB2	2.18	0.43
1:C:179:LEU:O	1:C:183:MET:HG3	2.18	0.43
1:A:92:HIS:CE1	1:A:95:GLU:HG3	2.53	0.43
1:E:32:THR:OG1	1:E:36:GLN:OE1	2.27	0.43
1:B:114:THR:HA	1:B:115:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:VAL:HG11	2:D:430:HOH:O	2.18	0.43
1:F:130:PRO:HA	2:F:414:HOH:O	2.18	0.43
1:C:142:VAL:HG11	1:C:235:ILE:HG23	2.01	0.43
1:B:6:ILE:O	1:B:10:LYS:HD3	2.18	0.43
1:A:5:LYS:HB3	1:A:5:LYS:HZ3	1.81	0.43
1:C:111:GLU:CD	1:C:111:GLU:H	2.22	0.43
1:B:13:GLU:O	1:B:17:ARG:HG3	2.18	0.43
1:C:281:ILE:HD11	1:C:294:ILE:HD12	2.01	0.43
1:A:66:ARG:HG2	1:A:89:ARG:CZ	2.48	0.43
1:A:30:ASP:HB2	1:A:278:GLY:HA2	2.00	0.43
1:E:319:ARG:CB	1:E:320:GLY:CA	2.94	0.43
1:A:26:GLY:HA2	2:A:427:HOH:O	2.18	0.43
1:F:124:LYS:HG2	1:F:131:PHE:CD2	2.54	0.43
1:F:283:LYS:HE3	1:F:318:MET:HB2	2.01	0.42
1:E:139:GLY:HA3	2:E:411:HOH:O	2.19	0.42
1:D:48:VAL:HG13	1:D:82:ILE:HD11	2.01	0.42
1:C:212:LEU:HB3	1:C:213:PRO:HD2	2.00	0.42
1:E:242:ILE:HG23	1:E:247:ARG:O	2.19	0.42
1:E:247:ARG:HG3	1:E:248:LEU:O	2.18	0.42
1:B:41:GLU:OE1	1:B:80:VAL:HB	2.19	0.42
1:B:233:GLU:O	1:B:236:TYR:HB3	2.19	0.42
1:F:33:ASN:OD1	1:F:36:GLN:N	2.40	0.42
1:F:317:PRO:O	1:F:318:MET:HG2	2.19	0.42
1:D:258:VAL:O	1:D:258:VAL:HG12	2.19	0.42
1:F:189:TYR:O	1:F:192:ALA:HB3	2.19	0.42
1:C:60:LYS:O	1:C:61:ALA:CB	2.66	0.42
1:D:134:GLY:HA2	1:D:153:ARG:O	2.19	0.42
1:F:120:PHE:CD1	1:F:223:TYR:CD1	3.07	0.42
1:F:20:ALA:C	1:F:22:MET:N	2.70	0.42
1:F:163:ILE:O	1:F:163:ILE:HG13	2.18	0.42
1:F:248:LEU:HA	1:F:249:PRO:HD3	1.85	0.42
1:B:312:ARG:O	1:B:313:GLU:O	2.37	0.42
1:B:53:LYS:HD3	1:B:54:VAL:H	1.85	0.42
1:F:277:VAL:HG11	1:F:294:ILE:HG21	2.00	0.42
1:C:215:ARG:CB	1:C:215:ARG:CZ	2.96	0.42
1:F:287:PRO:HD2	1:F:288:PRO:HD2	2.02	0.42
1:E:319:ARG:HD3	1:E:319:ARG:N	2.34	0.42
1:D:166:ALA:O	1:D:170:VAL:HG23	2.19	0.42
1:A:183:MET:CE	1:B:212:LEU:HD11	2.49	0.42
1:F:318:MET:HG3	1:F:318:MET:O	2.18	0.42
1:D:54:VAL:HG12	1:D:55:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG21	1:A:281:ILE:HD12	2.01	0.42
1:B:29:MET:HE3	1:B:281:ILE:CD1	2.50	0.42
1:C:106:MET:HE3	1:C:130:PRO:HB2	2.02	0.42
1:D:52:HIS:HD2	1:D:72:LYS:HG2	1.84	0.42
1:E:34:ALA:HB2	1:E:75:GLU:HG3	2.01	0.42
1:E:102:LEU:HD12	1:E:102:LEU:HA	1.86	0.41
1:C:39:ILE:H	1:C:39:ILE:HG12	1.57	0.41
1:C:287:PRO:CB	1:C:288:PRO:HD3	2.45	0.41
1:C:319:ARG:NH1	1:C:319:ARG:HG3	2.31	0.41
1:F:318:MET:CG	1:F:318:MET:O	2.69	0.41
1:D:316:GLU:HA	1:D:317:PRO:HD3	1.79	0.41
1:F:55:PRO:HB2	1:F:112:VAL:HG12	2.02	0.41
1:C:53:LYS:NZ	1:C:53:LYS:CB	2.84	0.41
1:D:181:GLN:NE2	1:D:246:GLY:CA	2.72	0.41
1:F:236:TYR:CE2	1:F:240:LEU:HD11	2.54	0.41
1:E:241:GLU:HG2	1:E:245:LEU:CD1	2.50	0.41
1:C:183:MET:HB3	1:C:187:GLU:OE1	2.21	0.41
1:E:146:TRP:CD1	1:E:234:ASP:HB3	2.55	0.41
1:F:157:GLU:HG2	1:F:160:THR:HG23	2.03	0.41
1:B:222:ILE:HA	1:B:222:ILE:HD12	1.67	0.41
1:E:57:ASP:O	1:E:60:LYS:CG	2.69	0.41
1:D:55:PRO:O	1:D:56:ALA:HB3	2.20	0.41
1:F:284:SER:HG	1:F:287:PRO:HG3	1.85	0.41
1:D:227:THR:HG23	1:D:229:ARG:H	1.86	0.41
1:B:314:ILE:N	1:B:314:ILE:HD13	2.34	0.41
1:E:279:SER:O	1:E:283:LYS:HB2	2.20	0.41
1:F:284:SER:OG	1:F:287:PRO:HG3	2.21	0.41
1:D:283:LYS:O	1:D:318:MET:HB3	2.20	0.41
1:D:168:ARG:HB2	1:E:118:PRO:HG3	2.03	0.41
1:C:21:LYS:HD3	2:C:419:HOH:O	2.20	0.41
1:C:34:ALA:HB2	1:C:75:GLU:HG3	2.02	0.41
1:E:244:LYS:HA	1:E:244:LYS:HD3	1.98	0.41
1:A:229:ARG:O	1:A:233:GLU:HG2	2.20	0.41
1:B:282:PHE:O	1:B:283:LYS:CB	2.68	0.41
1:D:72:LYS:HD2	1:D:75:GLU:OE1	2.21	0.41
1:E:197:GLU:N	1:E:198:PRO:CD	2.83	0.41
1:C:132:VAL:HA	1:C:151:MET:O	2.20	0.41
1:F:296:GLU:HB3	1:F:310:ILE:HD11	2.03	0.41
1:E:247:ARG:CG	1:E:248:LEU:N	2.83	0.41
1:A:124:LYS:CG	1:A:131:PHE:CD2	3.04	0.41
1:C:5:LYS:NZ	1:C:5:LYS:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LEU:HA	1:F:240:LEU:HD23	1.77	0.41
1:B:48:VAL:HG23	1:B:84:VAL:HG22	2.02	0.41
1:A:66:ARG:HD2	2:A:476:HOH:O	2.21	0.41
1:D:248:LEU:HD12	1:D:252:ASN:ND2	2.36	0.41
1:B:6:ILE:HG23	1:B:7:ILE:HG22	2.03	0.40
1:F:20:ALA:O	1:F:22:MET:N	2.54	0.40
1:E:123:TYR:CD2	1:E:224:GLU:HG2	2.55	0.40
1:B:27:VAL:CG2	1:B:298:VAL:HG21	2.51	0.40
1:C:283:LYS:HB2	1:C:283:LYS:HE2	1.92	0.40
1:A:32:THR:HA	1:A:51:LEU:O	2.22	0.40
1:A:82:ILE:HB	1:A:83:PRO:HD2	2.02	0.40
1:F:50:ALA:O	1:F:51:LEU:HD12	2.22	0.40
1:E:157:GLU:CG	1:E:160:THR:HG21	2.50	0.40
1:A:27:VAL:HG21	1:A:294:ILE:HG22	2.03	0.40
1:A:286:ASN:O	1:A:288:PRO:O	2.38	0.40
1:C:189:TYR:HA	1:C:236:TYR:CD1	2.56	0.40
1:A:254:ALA:HB2	1:A:267:MET:HE2	2.03	0.40
1:A:124:LYS:CG	1:A:131:PHE:CG	3.05	0.40
1:B:59:ARG:CD	1:B:60:LYS:HE3	2.52	0.40
1:F:163:ILE:HD13	1:F:263:ASP:HB3	2.03	0.40
1:C:285:SER:O	1:C:315:GLY:HA3	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	313/335 (93%)	302 (96%)	10 (3%)	1 (0%)	46 75
1	B	319/335 (95%)	299 (94%)	13 (4%)	7 (2%)	8 22
1	C	319/335 (95%)	294 (92%)	22 (7%)	3 (1%)	21 49
1	D	319/335 (95%)	307 (96%)	10 (3%)	2 (1%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	319/335 (95%)	308 (97%)	10 (3%)	1 (0%)	46 75
1	F	319/335 (95%)	294 (92%)	20 (6%)	5 (2%)	12 30
All	All	1908/2010 (95%)	1804 (94%)	85 (4%)	19 (1%)	19 45

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	283	LYS
1	B	313	GLU
1	C	61	ALA
1	C	316	GLU
1	A	284	SER
1	B	280	GLY
1	C	318	MET
1	E	319	ARG
1	F	282	PHE
1	B	58	ILE
1	B	281	ILE
1	D	278	GLY
1	F	3	LYS
1	F	279	SER
1	B	60	LYS
1	F	318	MET
1	D	185	ASP
1	F	104	VAL
1	B	286	ASN

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	249/267 (93%)	236 (95%)	13 (5%)	29 58
1	B	254/267 (95%)	224 (88%)	30 (12%)	6 15
1	C	254/267 (95%)	242 (95%)	12 (5%)	32 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	254/267 (95%)	235 (92%)	19 (8%)	17 38
1	E	254/267 (95%)	233 (92%)	21 (8%)	14 31
1	F	254/267 (95%)	237 (93%)	17 (7%)	20 44
All	All	1519/1602 (95%)	1407 (93%)	112 (7%)	17 39

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	15	LEU
1	A	35	GLU
1	A	51	LEU
1	A	53	LYS
1	A	74	GLN
1	A	93	GLU
1	A	113	LEU
1	A	124	LYS
1	A	281	ILE
1	A	292	ARG
1	A	305	ASP
1	A	313	GLU
1	B	2	ASP
1	B	3	LYS
1	B	5	LYS
1	B	7	ILE
1	B	8	MET
1	B	9	GLU
1	B	15	LEU
1	B	19	PHE
1	B	48	VAL
1	B	51	LEU
1	B	53	LYS
1	B	57	ASP
1	B	59	ARG
1	B	60	LYS
1	B	70	VAL
1	B	72	LYS
1	B	126	LYS
1	B	222	ILE
1	B	227	THR
1	B	239	LEU

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Mol	Chain	Res	Type
1	B	245	LEU
1	B	277	VAL
1	B	284	SER
1	B	292	ARG
1	B	302	ASP
1	B	305	ASP
1	B	313	GLU
1	B	314	ILE
1	B	318	MET
1	B	319	ARG
1	C	8	MET
1	C	21	LYS
1	C	35	GLU
1	C	39	ILE
1	C	51	LEU
1	C	60	LYS
1	C	75	GLU
1	C	222	ILE
1	C	229	ARG
1	C	292	ARG
1	C	316	GLU
1	C	321	GLN
1	D	4	LEU
1	D	35	GLU
1	D	54	VAL
1	D	60	LYS
1	D	85	MET
1	D	110	SER
1	D	113	LEU
1	D	180	ILE
1	D	212	LEU
1	D	214	LYS
1	D	222	ILE
1	D	224	GLU
1	D	233	GLU
1	D	279	SER
1	D	296	GLU
1	D	313	GLU
1	D	314	ILE
1	D	316	GLU
1	D	318	MET
1	E	7	ILE

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Mol	Chain	Res	Type
1	E	8	MET
1	E	14	ARG
1	E	15	LEU
1	E	22	MET
1	E	42	GLU
1	E	51	LEU
1	E	59	ARG
1	E	60	LYS
1	E	67	MET
1	E	72	LYS
1	E	113	LEU
1	E	128	THR
1	E	218	GLU
1	E	222	ILE
1	E	233	GLU
1	E	289	LYS
1	E	292	ARG
1	E	314	ILE
1	E	319	ARG
1	E	321	GLN
1	F	3	LYS
1	F	8	MET
1	F	9	GLU
1	F	22	MET
1	F	38	ARG
1	F	59	ARG
1	F	72	LYS
1	F	76	ILE
1	F	110	SER
1	F	113	LEU
1	F	275	VAL
1	F	282	PHE
1	F	283	LYS
1	F	284	SER
1	F	285	SER
1	F	292	ARG
1	F	319	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	ASN

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Mol	Chain	Res	Type
1	C	286	ASN
1	C	321	GLN
1	D	52	HIS
1	D	181	GLN
1	E	52	HIS
1	E	121	HIS
1	E	286	ASN
1	F	52	HIS

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

There are no ligands in this entry.

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	315/335 (94%)	-0.51	0 100 100	29, 41, 64, 88	0
1	B	321/335 (95%)	-0.28	10 (3%) 52 52	31, 49, 99, 125	0
1	C	321/335 (95%)	-0.15	14 (4%) 38 37	38, 54, 94, 123	0
1	D	321/335 (95%)	-0.35	7 (2%) 65 66	32, 50, 90, 139	0
1	E	321/335 (95%)	-0.43	3 (0%) 85 86	27, 42, 70, 82	0
1	F	321/335 (95%)	-0.28	6 (1%) 70 70	32, 51, 91, 113	0
All	All	1920/2010 (95%)	-0.33	40 (2%) 67 68	27, 48, 89, 139	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	315	GLY	8.4
1	B	58	ILE	7.1
1	C	317	PRO	6.4
1	F	322	ALA	5.3
1	D	3	LYS	5.0
1	C	316	GLU	4.6
1	D	322	ALA	4.6
1	C	319	ARG	4.5
1	B	285	SER	4.3
1	E	322	ALA	4.2
1	C	322	ALA	4.1
1	B	322	ALA	4.0
1	D	2	ASP	3.9
1	F	282	PHE	3.8
1	B	2	ASP	3.8
1	B	3	LYS	3.4
1	B	319	ARG	3.2
1	B	280	GLY	3.1
1	D	4	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	321	GLN	3.0
1	C	282	PHE	3.0
1	B	315	GLY	2.9
1	C	283	LYS	2.9
1	C	320	GLY	2.8
1	E	321	GLN	2.7
1	C	321	GLN	2.7
1	F	2	ASP	2.7
1	B	314	ILE	2.6
1	D	61	ALA	2.5
1	F	321	GLN	2.5
1	C	8	MET	2.4
1	F	4	LEU	2.4
1	C	2	ASP	2.2
1	C	218	GLU	2.2
1	F	319	ARG	2.1
1	E	319	ARG	2.1
1	B	42	GLU	2.1
1	D	8	MET	2.1
1	C	318	MET	2.1
1	C	313	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 carbohydrates 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.