Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:06 AM GMT

PDB ID	:	3NNK
Title	:	Biochemical and Structural Characterization of a Ureidoglycine Aminotransferase in the Klebsiella pneumoniae Uric Acid Catabolic Pathway
Authors	:	French, J.B.; Ealick, S.E.
Deposited on	:	2010-06-23
Resolution	:	2.58 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:

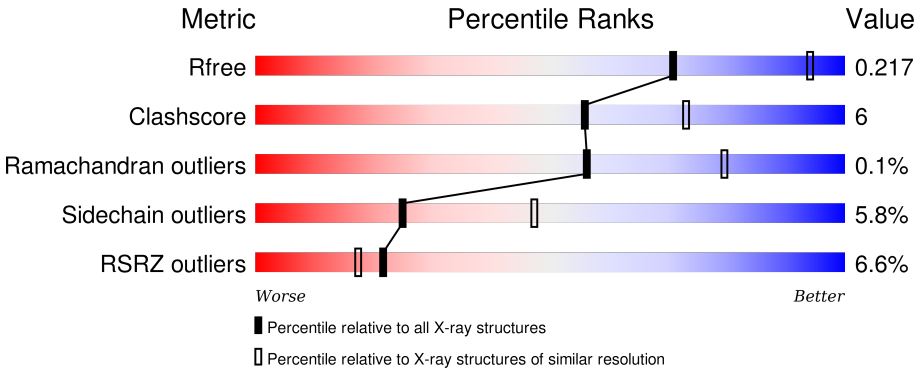
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.58 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	411	11% 81% 17%
1	B	411	10% 79% 19%
1	C	411	8% 81% 17%
1	D	411	3% 79% 19%
1	E	411	6% 80% 19%

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Mol	Chain	Length	Quality of chain
1	F	411	6% 81% 18%
1	G	411	10% 79% 19%
1	H	411	5% 82% 16%
1	J	411	5% 82% 17%
1	K	411	9% 86% 13%
1	L	411	7% 82% 15%
1	M	411	4% 80% 19%
1	O	411	2% 84% 15%
1	P	411	5% 81% 19%
1	R	411	9% 80% 19%
1	S	411	6% 81% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 51634 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 Ureidoglycine-glyoxylate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	P	S	0	0	0
			3158	1987	558	586	1	26			
1	B	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	C	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	D	410	Total	C	N	O	P	S	0	0	0
			3180	1999	567	588	1	25			
1	E	410	Total	C	N	O	P	S	0	0	0
			3147	1981	557	583	1	25			
1	F	410	Total	C	N	O	P	S	0	0	0
			3171	1994	566	585	1	25			
1	G	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	H	410	Total	C	N	O	P	S	0	0	0
			3183	2000	567	590	1	25			
1	J	410	Total	C	N	O	P	S	0	0	0
			3154	1984	558	586	1	25			
1	K	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	L	409	Total	C	N	O	P	S	0	0	0
			3156	1982	564	584	1	25			
1	M	410	Total	C	N	O	P	S	0	0	0
			3183	2000	567	590	1	25			
1	O	410	Total	C	N	O	P	S	0	0	0
			3154	1984	558	586	1	25			
1	P	410	Total	C	N	O	P	S	0	0	0
			3175	1996	567	586	1	25			
1	R	410	Total	C	N	O	P	S	0	0	0
			3164	1988	565	585	1	25			
1	S	410	Total	C	N	O	P	S	0	0	0
			3179	1999	567	587	1	25			

- Molecule 2 is water.

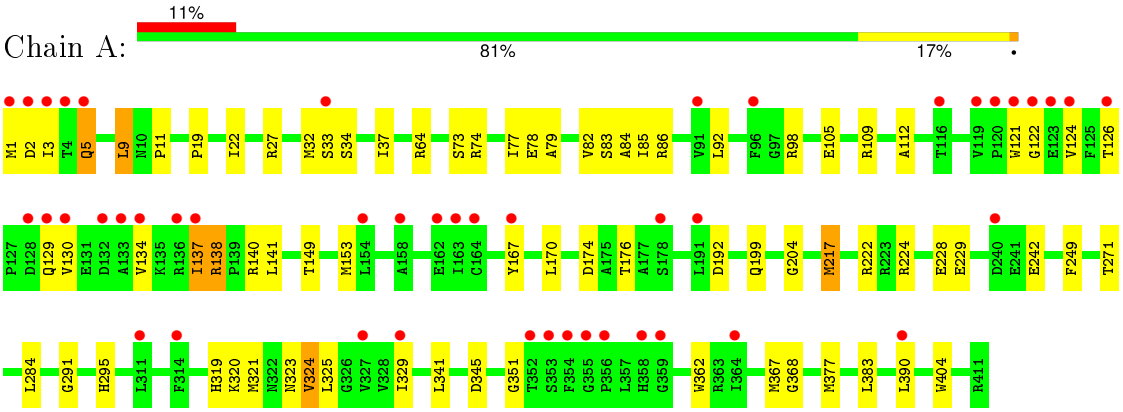
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	51	Total O 51 51	0	0
2	C	39	Total O 39 39	0	0
2	D	33	Total O 33 33	0	0
2	E	49	Total O 49 49	0	0
2	F	73	Total O 73 73	0	0
2	G	66	Total O 66 66	0	0
2	H	59	Total O 59 59	0	0
2	J	73	Total O 73 73	0	0
2	K	71	Total O 71 71	0	0
2	L	64	Total O 64 64	0	0
2	M	59	Total O 59 59	0	0
2	O	69	Total O 69 69	0	0
2	P	76	Total O 76 76	0	0
2	R	69	Total O 69 69	0	0
2	S	60	Total O 60 60	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.

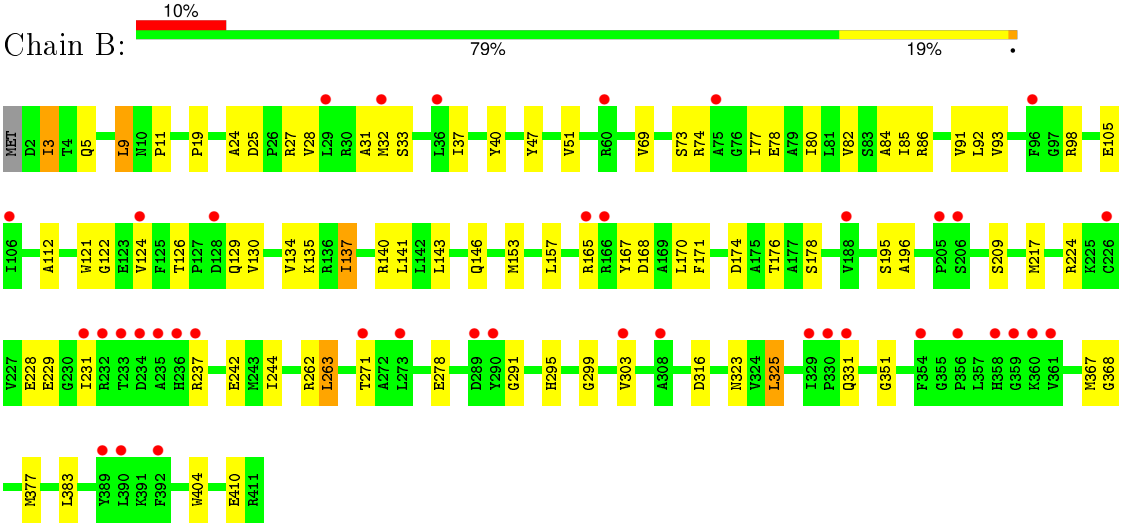
- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain A:



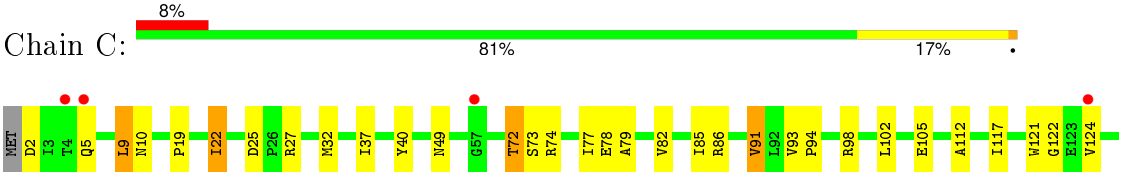
- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

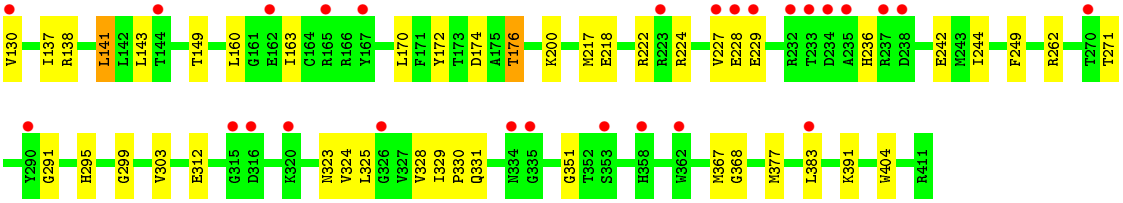
Chain B:



- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

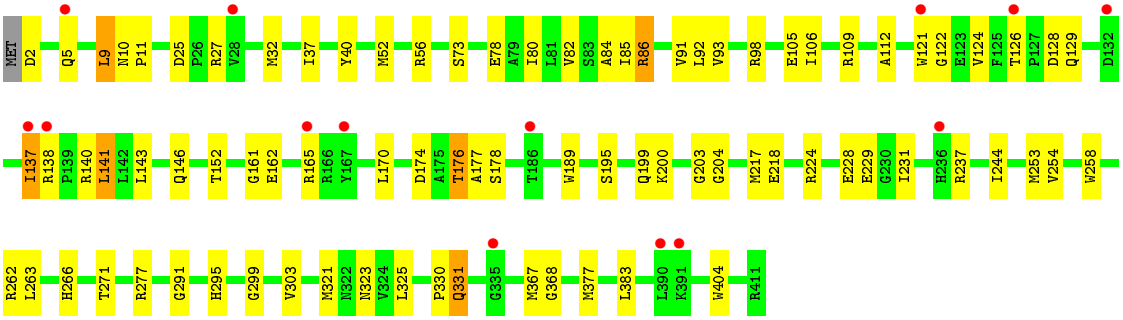
Chain C:





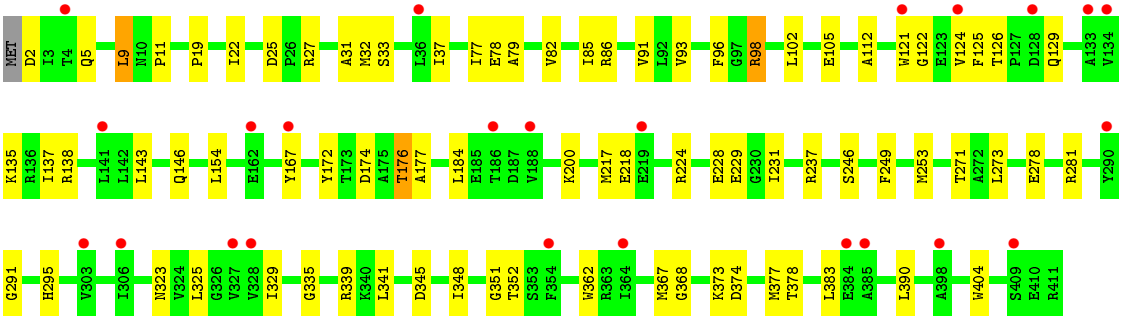
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain D:



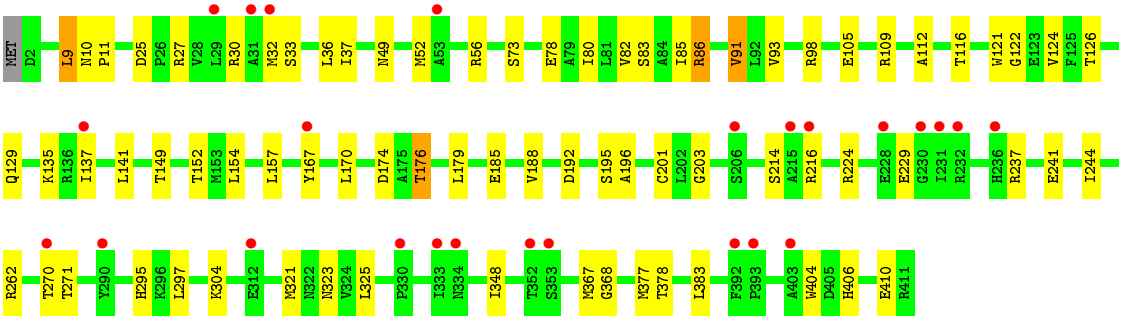
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain E:



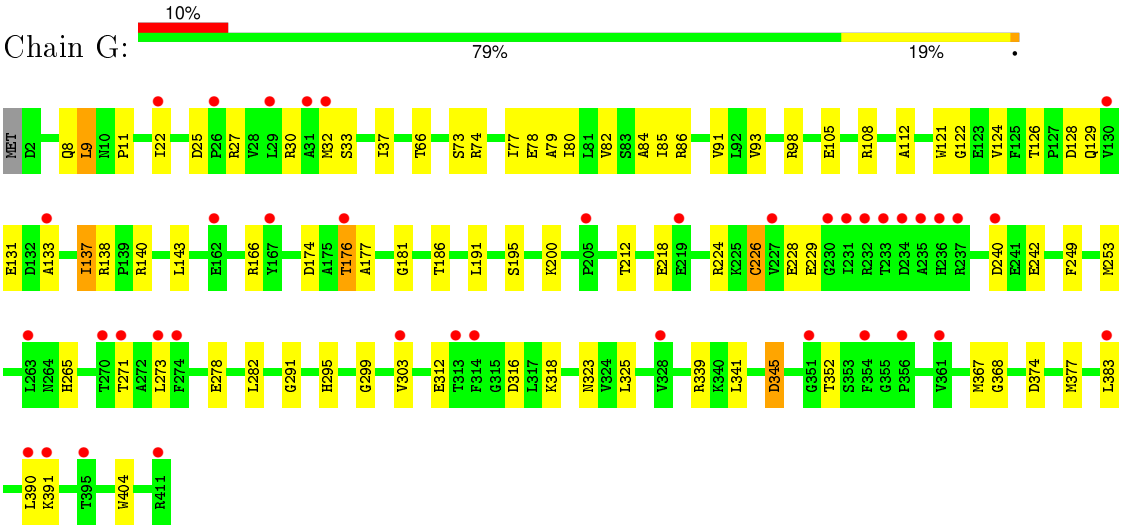
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain F:



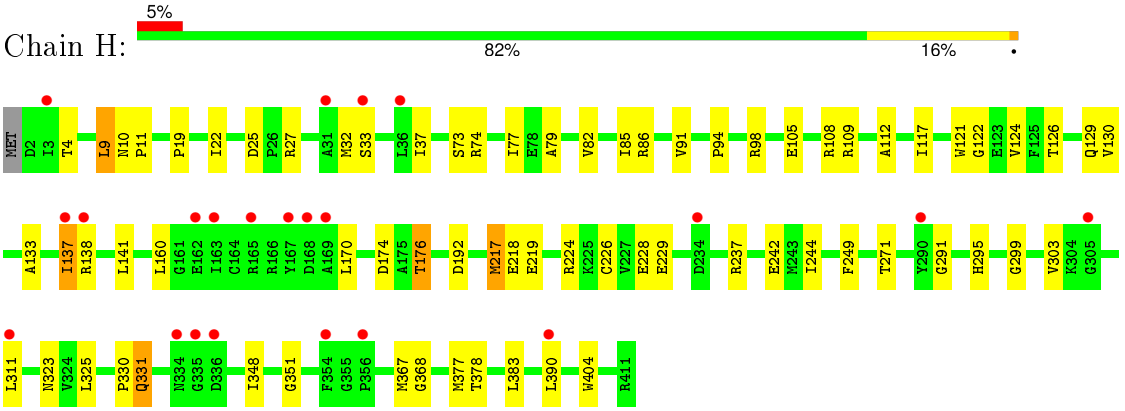
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain G:



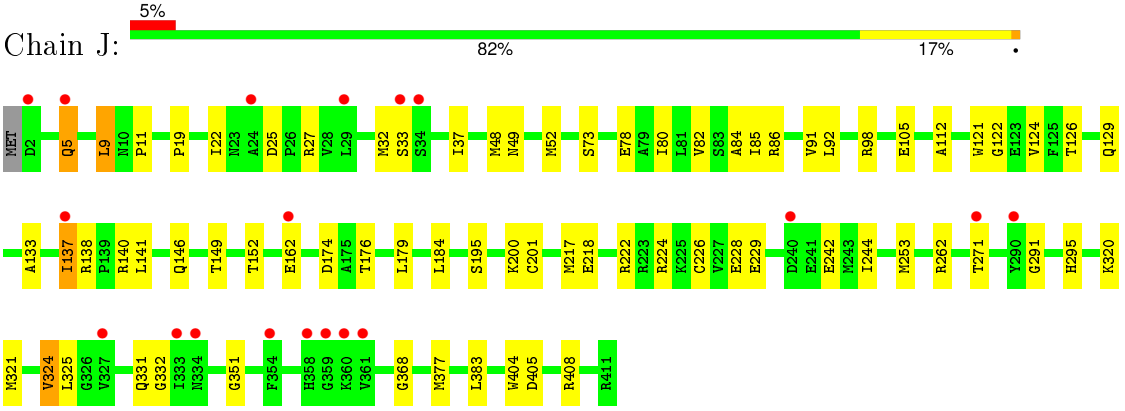
- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain H:



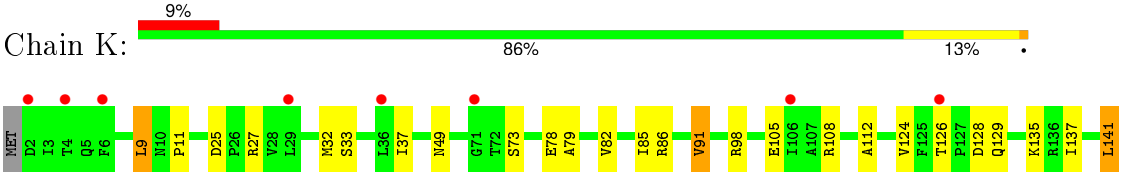
- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

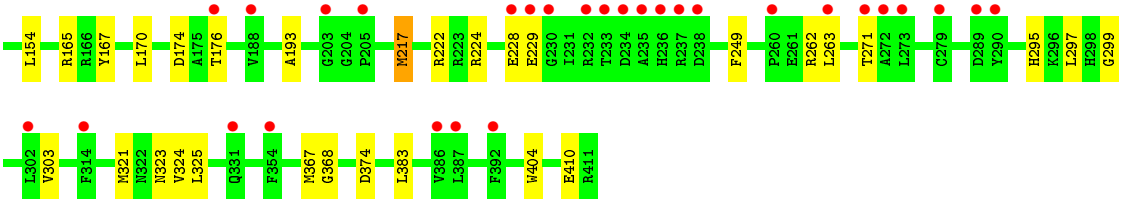
Chain J:



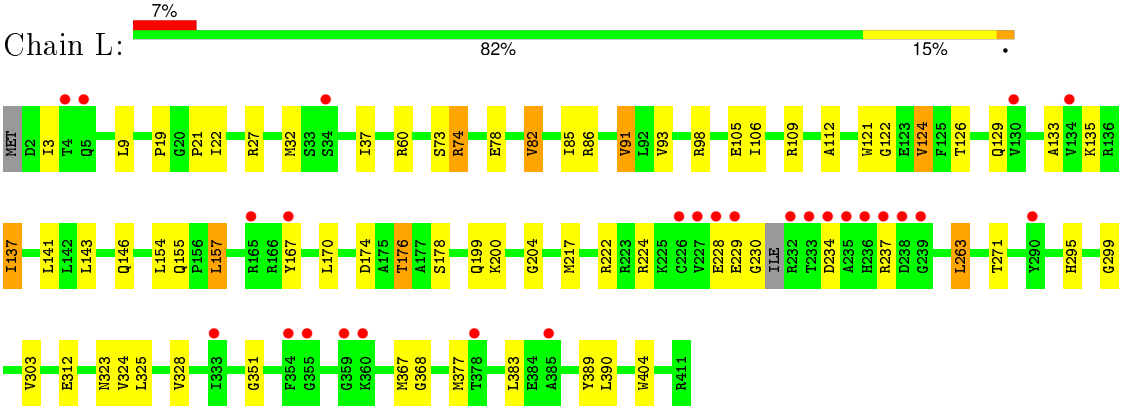
- Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain K:

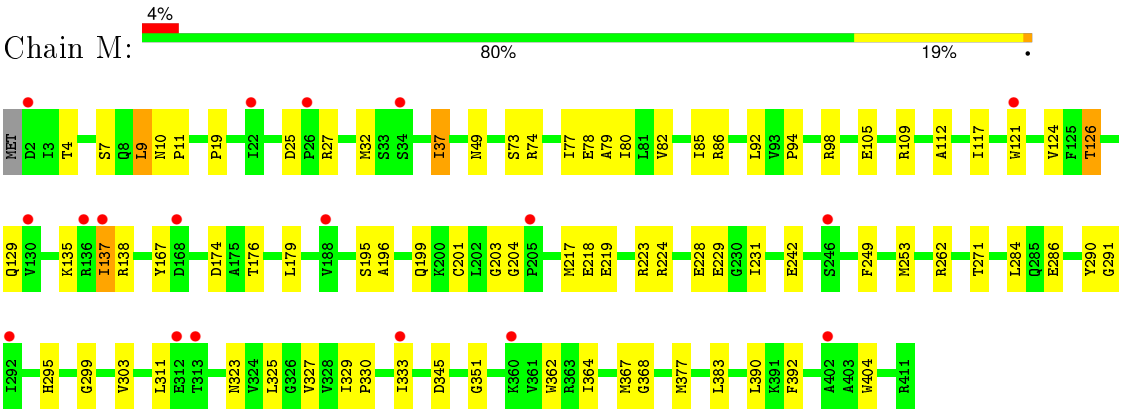




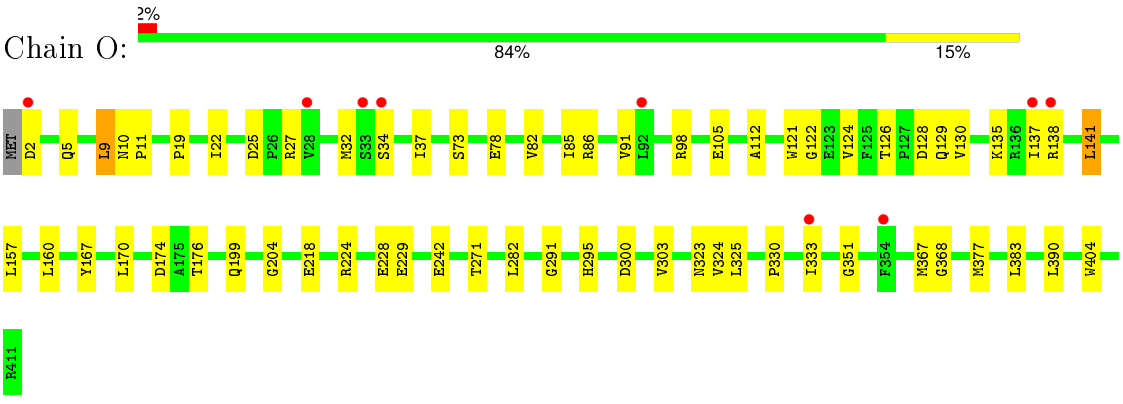
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase



• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

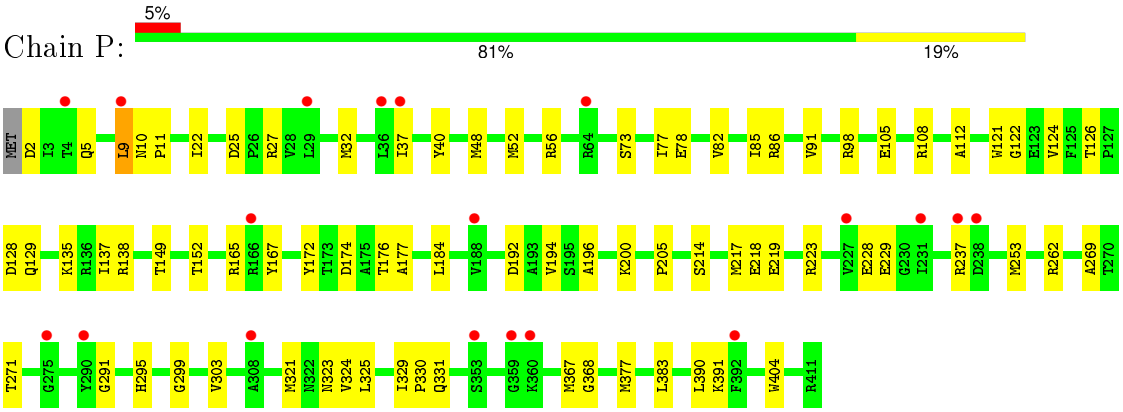


• Molecule 1: Ureidoglycine-glyoxylate aminotransferase



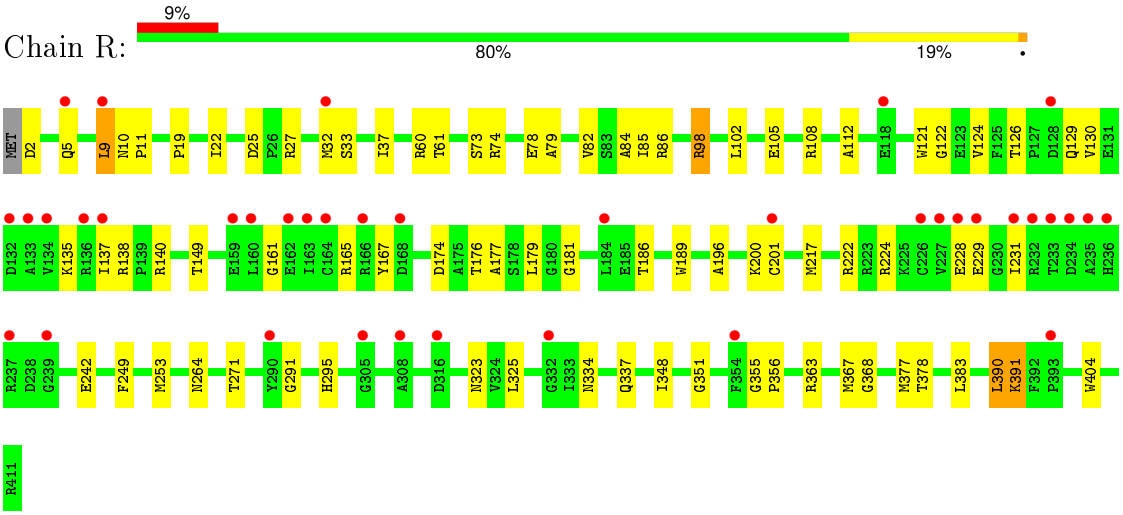
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain P:



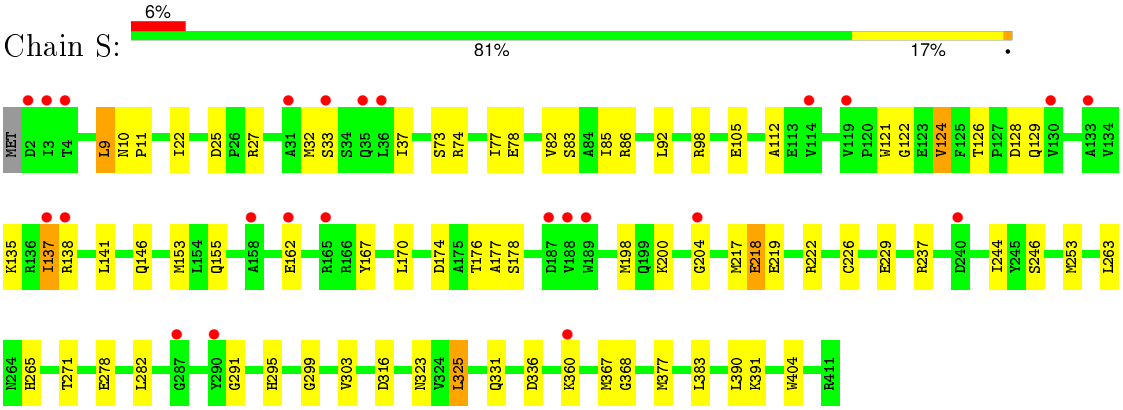
• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain R:



• Molecule 1: Ureidoglycine-glyoxylate aminotransferase

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	142.15Å 149.20Å 198.00Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.58 49.85 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.58) 93.9 (49.85-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.246 0.192 , 0.217	Depositor DCC
R_{free} test set	12155 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.5	EDS
Estimated twinning fraction	0.549 for H, K, L 0.451 for H, -K, -L 0.046 for -k,-h,-l 0.048 for k,h,-l 0.420 for h,-k,-l	Xtriage
Reported twinning fraction	0.549 for H, K, L 0.451 for H, -K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	2 of 242432 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	51634	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% 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: LLP

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	0.31	0/3198	0.52	0/4335
1	B	0.31	0/3215	0.51	0/4354
1	C	0.31	0/3204	0.52	1/4341 (0.0%)
1	D	0.32	0/3220	0.52	1/4360 (0.0%)
1	E	0.31	0/3187	0.51	0/4321
1	F	0.31	0/3211	0.52	0/4349
1	G	0.31	0/3204	0.51	0/4341
1	H	0.31	0/3223	0.51	0/4364
1	J	0.31	0/3194	0.52	0/4330
1	K	0.31	0/3215	0.52	2/4354 (0.0%)
1	L	0.31	0/3195	0.52	1/4327 (0.0%)
1	M	0.32	0/3223	0.51	0/4364
1	O	0.31	0/3194	0.52	1/4330 (0.0%)
1	P	0.31	0/3215	0.53	0/4354
1	R	0.31	0/3204	0.51	0/4341
1	S	0.32	0/3219	0.51	0/4358
All	All	0.31	0/51321	0.52	6/69523 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	141	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	141	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	141	LEU	CA-CB-CG	5.22	127.31	115.30
1	L	263	LEU	CA-CB-CG	5.14	127.13	115.30
1	O	141	LEU	CA-CB-CG	5.03	126.87	115.30
1	K	263	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3158	0	3092	45	0
1	B	3175	0	3129	51	0
1	C	3164	0	3103	46	0
1	D	3180	0	3135	52	0
1	E	3147	0	3078	41	0
1	F	3171	0	3123	47	0
1	G	3164	0	3103	52	0
1	H	3183	0	3137	45	0
1	J	3154	0	3086	42	0
1	K	3175	0	3129	35	0
1	L	3156	0	3091	40	0
1	M	3183	0	3137	47	0
1	O	3154	0	3086	36	0
1	P	3175	0	3129	45	0
1	R	3164	0	3103	45	0
1	S	3179	0	3135	46	0
2	A	41	0	0	0	0
2	B	51	0	0	3	0
2	C	39	0	0	1	0
2	D	33	0	0	0	0
2	E	49	0	0	0	0
2	F	73	0	0	2	0
2	G	66	0	0	2	0
2	H	59	0	0	0	0
2	J	73	0	0	0	0
2	K	71	0	0	0	0
2	L	64	0	0	0	0
2	M	59	0	0	0	0
2	O	69	0	0	0	0
2	P	76	0	0	3	0
2	R	69	0	0	0	0
2	S	60	0	0	0	0
All	All	51634	0	49796	626	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 6.

All (626) 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:72:THR:HG23	1:C:200:LLP:OP2	1.58	1.03
1:H:126:THR:H	1:H:129:GLN:HE21	1.14	0.96
1:K:174:ASP:OD1	1:K:176:THR:HG23	1.69	0.92
1:O:295:HIS:HE1	1:O:368:GLY:H	1.14	0.91
1:K:9:LEU:HD13	1:K:11:PRO:HD3	1.53	0.90
1:B:174:ASP:OD1	1:B:176:THR:HG23	1.72	0.89
1:K:126:THR:H	1:K:129:GLN:HE21	1.21	0.88
1:J:9:LEU:HD13	1:J:11:PRO:HD3	1.57	0.86
1:D:174:ASP:OD1	1:D:176:THR:HG23	1.77	0.85
1:G:295:HIS:HE1	1:G:368:GLY:H	1.25	0.83
1:O:126:THR:H	1:O:129:GLN:HE21	1.27	0.81
1:C:72:THR:CG2	1:C:200:LLP:OP2	2.29	0.81
1:R:390:LEU:O	1:R:391:LYS:HB2	1.80	0.80
1:M:25:ASP:OD1	1:M:27:ARG:HD3	1.80	0.80
1:S:78:GLU:O	1:S:82:VAL:HG23	1.81	0.79
1:J:174:ASP:OD1	1:J:176:THR:HG23	1.83	0.79
1:J:85:ILE:HG21	1:J:112:ALA:HB2	1.64	0.79
1:L:78:GLU:O	1:L:82:VAL:HG23	1.82	0.78
1:A:32:MET:SD	1:B:271:THR:HG21	2.23	0.78
1:E:85:ILE:HG21	1:E:112:ALA:HB2	1.66	0.78
1:J:229:GLU:H	1:K:105:GLU:HG3	1.50	0.77
1:S:174:ASP:OD1	1:S:176:THR:HG23	1.84	0.77
1:K:78:GLU:O	1:K:82:VAL:HG23	1.84	0.77
1:O:174:ASP:OD1	1:O:176:THR:HG23	1.85	0.77
1:C:295:HIS:HE1	1:C:368:GLY:H	1.29	0.76
1:F:295:HIS:HE1	1:F:368:GLY:H	1.30	0.76
1:J:295:HIS:HE1	1:J:368:GLY:H	1.32	0.75
1:J:32:MET:SD	1:K:271:THR:HG21	2.26	0.75
1:G:174:ASP:OD1	1:G:176:THR:HG23	1.88	0.73
1:M:295:HIS:HE1	1:M:368:GLY:H	1.34	0.73
1:F:297:LEU:HD13	1:F:410:GLU:HG2	1.69	0.73
1:G:9:LEU:HD13	1:G:11:PRO:HD3	1.70	0.73
1:G:78:GLU:O	1:G:82:VAL:HG23	1.89	0.73
1:O:330:PRO:HG2	1:O:333:ILE:HG13	1.69	0.73
1:J:105:GLU:HG3	1:K:229:GLU:H	1.52	0.73
1:B:323:ASN:HB2	1:B:367:MET:HG2	1.71	0.72
1:E:174:ASP:OD1	1:E:176:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ILE:HG21	1:F:112:ALA:HB2	1.71	0.72
1:A:73:SER:HB3	1:A:176:THR:HG21	1.72	0.72
1:A:85:ILE:HG21	1:A:112:ALA:HB2	1.69	0.72
1:H:9:LEU:HD13	1:H:11:PRO:HD3	1.70	0.72
1:P:295:HIS:HE1	1:P:368:GLY:H	1.34	0.72
1:B:25:ASP:OD1	1:B:27:ARG:HD3	1.90	0.71
1:F:126:THR:H	1:F:129:GLN:HE21	1.38	0.71
1:C:229:GLU:H	1:D:105:GLU:HG3	1.54	0.71
1:P:85:ILE:HG21	1:P:112:ALA:HB2	1.72	0.71
1:A:295:HIS:HE1	1:A:368:GLY:H	1.38	0.71
1:O:295:HIS:HE1	1:O:368:GLY:N	1.89	0.70
1:R:229:GLU:H	1:S:105:GLU:HG3	1.54	0.70
1:A:9:LEU:HD13	1:A:11:PRO:HD3	1.73	0.70
1:C:174:ASP:OD1	1:C:176:THR:HG23	1.92	0.70
1:R:32:MET:SD	1:S:271:THR:HG21	2.32	0.69
1:L:174:ASP:OD1	1:L:176:THR:HG23	1.93	0.69
1:K:295:HIS:HE1	1:K:368:GLY:H	1.40	0.69
1:B:126:THR:H	1:B:129:GLN:HE21	1.41	0.69
1:A:229:GLU:H	1:B:105:GLU:HG3	1.57	0.69
1:E:105:GLU:HG3	1:F:229:GLU:H	1.57	0.69
1:A:291:GLY:O	1:A:295:HIS:HD2	1.76	0.69
1:M:126:THR:H	1:M:129:GLN:HE21	1.39	0.69
1:D:82:VAL:HG12	1:D:244:ILE:HG23	1.73	0.68
1:K:323:ASN:HB2	1:K:367:MET:HG2	1.73	0.68
1:K:85:ILE:HG21	1:K:112:ALA:HB2	1.75	0.68
1:G:229:GLU:H	1:H:105:GLU:HG3	1.58	0.68
1:C:85:ILE:HG21	1:C:112:ALA:HB2	1.75	0.68
1:P:174:ASP:OD1	1:P:176:THR:HG23	1.94	0.68
1:B:295:HIS:HE1	1:B:368:GLY:H	1.42	0.67
1:H:295:HIS:HE1	1:H:368:GLY:H	1.43	0.67
1:R:126:THR:H	1:R:129:GLN:HE21	1.43	0.67
1:R:105:GLU:HG3	1:S:229:GLU:H	1.59	0.67
1:R:84:ALA:O	1:R:140:ARG:NH1	2.28	0.67
1:P:25:ASP:OD1	1:P:27:ARG:HD3	1.93	0.67
1:B:73:SER:HB3	1:B:176:THR:HG21	1.77	0.67
1:D:295:HIS:HE1	1:D:368:GLY:H	1.41	0.67
1:L:323:ASN:HB2	1:L:367:MET:HG2	1.77	0.66
1:R:174:ASP:OD1	1:R:176:THR:HG23	1.95	0.66
1:H:224:ARG:HD2	1:H:242:GLU:O	1.95	0.66
1:M:78:GLU:O	1:M:82:VAL:HG23	1.95	0.66
1:C:105:GLU:HG3	1:D:229:GLU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:295:HIS:CE1	1:J:368:GLY:H	2.13	0.66
1:A:271:THR:HG21	1:B:32:MET:SD	2.36	0.66
1:K:141:LEU:HD13	1:K:170:LEU:HB2	1.78	0.66
1:E:9:LEU:HD13	1:E:11:PRO:HD3	1.78	0.66
1:K:126:THR:H	1:K:129:GLN:NE2	1.94	0.66
1:E:229:GLU:H	1:F:105:GLU:HG3	1.60	0.66
1:D:126:THR:H	1:D:129:GLN:HE21	1.44	0.65
1:B:3:ILE:HG13	1:B:3:ILE:O	1.94	0.65
1:G:291:GLY:O	1:G:295:HIS:HD2	1.79	0.65
1:M:291:GLY:O	1:M:295:HIS:HD2	1.78	0.65
1:R:271:THR:HG21	1:S:32:MET:SD	2.37	0.65
1:O:229:GLU:H	1:P:105:GLU:HG3	1.60	0.65
1:R:25:ASP:OD1	1:R:27:ARG:HD3	1.96	0.65
1:O:295:HIS:CE1	1:O:368:GLY:H	2.05	0.64
1:M:174:ASP:OD1	1:M:176:THR:HG23	1.97	0.64
1:D:85:ILE:HG21	1:D:112:ALA:HB2	1.79	0.64
1:R:85:ILE:HG21	1:R:112:ALA:HB2	1.79	0.64
1:S:73:SER:HB3	1:S:176:THR:HG21	1.78	0.64
1:O:228:GLU:HG2	1:P:105:GLU:HG3	1.79	0.64
1:D:177:ALA:HA	1:D:200:LLP:HG2	1.78	0.64
1:E:126:THR:H	1:E:129:GLN:HE21	1.45	0.64
1:S:126:THR:H	1:S:129:GLN:HE21	1.45	0.64
1:B:291:GLY:O	1:B:295:HIS:HD2	1.81	0.64
1:S:85:ILE:HG21	1:S:112:ALA:HB2	1.79	0.64
1:S:9:LEU:HD13	1:S:11:PRO:HD3	1.79	0.63
1:L:105:GLU:HG3	1:M:228:GLU:HG2	1.79	0.63
1:J:73:SER:HB3	1:J:176:THR:HG21	1.80	0.63
1:F:295:HIS:CE1	1:F:368:GLY:H	2.15	0.63
1:H:126:THR:H	1:H:129:GLN:NE2	1.94	0.63
1:J:271:THR:HG21	1:K:32:MET:SD	2.39	0.63
1:E:295:HIS:HE1	1:E:368:GLY:H	1.47	0.63
1:L:135:LYS:HE3	1:L:167:TYR:OH	1.98	0.62
1:O:323:ASN:HB2	1:O:367:MET:HG2	1.82	0.62
1:F:323:ASN:HB2	1:F:367:MET:HG2	1.80	0.62
1:P:135:LYS:HE3	1:P:167:TYR:OH	1.99	0.62
1:F:174:ASP:OD1	1:F:176:THR:HG23	1.98	0.62
1:R:231:ILE:HD13	1:R:264:ASN:O	2.00	0.62
1:G:32:MET:SD	1:H:271:THR:HG21	2.39	0.61
1:R:295:HIS:HE1	1:R:368:GLY:H	1.47	0.61
1:C:323:ASN:HB2	1:C:367:MET:HG2	1.81	0.61
1:A:33:SER:HB3	1:B:33:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:SER:HB3	1:F:176:THR:HG21	1.83	0.61
1:A:284:LEU:HB2	1:B:3:ILE:HD13	1.82	0.61
1:P:73:SER:HB3	1:P:176:THR:HG21	1.81	0.61
1:B:85:ILE:HG21	1:B:112:ALA:HB2	1.82	0.61
1:C:2:ASP:O	1:C:5:GLN:HG2	2.01	0.61
1:A:295:HIS:CE1	1:A:368:GLY:H	2.19	0.61
1:M:295:HIS:CE1	1:M:368:GLY:H	2.16	0.61
1:M:333:ILE:HD11	1:M:392:PHE:HB2	1.82	0.61
1:G:105:GLU:HG3	1:H:229:GLU:H	1.66	0.60
1:H:85:ILE:HG21	1:H:112:ALA:HB2	1.83	0.60
1:M:176:THR:HG22	1:M:196:ALA:HA	1.82	0.60
1:L:295:HIS:HE1	1:L:368:GLY:H	1.47	0.60
1:K:25:ASP:OD1	1:K:27:ARG:HD3	2.01	0.60
1:M:323:ASN:HB2	1:M:367:MET:HG2	1.83	0.60
1:L:271:THR:HG21	1:M:32:MET:SD	2.41	0.60
1:S:295:HIS:CE1	1:S:368:GLY:H	2.19	0.60
1:D:141:LEU:HD13	1:D:170:LEU:HB2	1.84	0.60
1:A:105:GLU:HG3	1:B:229:GLU:H	1.65	0.60
1:F:304:LYS:HD2	1:F:406:HIS:HB2	1.84	0.60
1:G:224:ARG:HD2	1:G:242:GLU:O	2.02	0.59
1:E:373:LYS:HG2	2:G:921:HOH:O	2.01	0.59
1:G:295:HIS:HE1	1:G:368:GLY:N	1.98	0.59
1:L:85:ILE:HG21	1:L:112:ALA:HB2	1.84	0.59
1:L:229:GLU:H	1:M:105:GLU:HG3	1.66	0.59
1:M:85:ILE:HG21	1:M:112:ALA:HB2	1.84	0.59
1:O:25:ASP:OD1	1:O:27:ARG:HD3	2.02	0.59
1:S:295:HIS:HE1	1:S:368:GLY:H	1.50	0.59
1:L:74:ARG:HD2	1:L:200:LLP:OP2	2.01	0.59
1:L:73:SER:HB3	1:L:176:THR:HG21	1.83	0.59
1:L:228:GLU:HG2	1:L:230:GLY:H	1.67	0.59
1:P:149:THR:HG22	1:P:324:VAL:HG21	1.84	0.59
1:P:295:HIS:CE1	1:P:368:GLY:H	2.18	0.59
1:P:126:THR:H	1:P:129:GLN:HE21	1.50	0.59
1:J:84:ALA:O	1:J:140:ARG:NH1	2.36	0.59
1:C:295:HIS:CE1	1:C:368:GLY:H	2.17	0.59
1:J:152:THR:HA	1:J:321:MET:HE3	1.85	0.59
1:E:271:THR:HG21	1:F:32:MET:SD	2.42	0.59
1:R:177:ALA:HA	1:R:200:LLP:HG3	1.85	0.59
1:M:73:SER:HB3	1:M:176:THR:HG21	1.85	0.58
1:P:2:ASP:O	1:P:5:GLN:HG2	2.03	0.58
1:A:323:ASN:HB2	1:A:367:MET:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:MET:SD	1:P:271:THR:HG21	2.44	0.58
1:G:228:GLU:HG2	1:H:105:GLU:HG3	1.84	0.58
1:P:323:ASN:HB2	1:P:367:MET:HG2	1.85	0.58
1:R:323:ASN:HB2	1:R:367:MET:HG2	1.84	0.58
1:R:33:SER:HB3	1:S:33:SER:HB3	1.85	0.58
1:J:226:CYS:SG	1:K:108:ARG:NH1	2.75	0.58
1:K:154:LEU:HD23	1:K:321:MET:HG2	1.86	0.58
1:O:126:THR:H	1:O:129:GLN:NE2	2.00	0.58
1:B:295:HIS:HE1	1:B:368:GLY:N	2.02	0.58
1:P:27:ARG:HD2	1:S:10:ASN:ND2	2.19	0.58
1:E:32:MET:SD	1:F:271:THR:HG21	2.44	0.58
1:D:323:ASN:HB2	1:D:367:MET:HG2	1.84	0.58
1:G:85:ILE:HG21	1:G:112:ALA:HB2	1.84	0.57
1:D:78:GLU:O	1:D:82:VAL:HG23	2.04	0.57
1:F:25:ASP:OD1	1:F:27:ARG:HD3	2.04	0.57
1:H:330:PRO:O	1:H:331:GLN:CB	2.52	0.57
1:O:130:VAL:HG21	1:O:160:LEU:HG	1.85	0.57
1:P:330:PRO:O	1:P:331:GLN:HB2	2.04	0.57
1:C:271:THR:HG21	1:D:32:MET:SD	2.44	0.57
1:E:291:GLY:O	1:E:295:HIS:HD2	1.87	0.57
1:F:135:LYS:HE3	1:F:167:TYR:OH	2.04	0.57
1:O:78:GLU:O	1:O:82:VAL:HG23	2.03	0.57
1:O:105:GLU:HG3	1:P:228:GLU:HG2	1.86	0.57
1:E:135:LYS:HE3	1:E:167:TYR:OH	2.04	0.57
1:B:135:LYS:HE3	1:B:167:TYR:OH	2.04	0.57
1:P:126:THR:H	1:P:129:GLN:NE2	2.03	0.57
1:G:271:THR:HG21	1:H:32:MET:SD	2.45	0.57
1:D:25:ASP:OD1	1:D:27:ARG:HD3	2.04	0.57
1:E:79:ALA:HA	1:E:249:PHE:HB3	1.87	0.57
1:C:72:THR:HG21	1:D:266:HIS:HB2	1.87	0.56
1:B:40:TYR:HE1	1:B:262:ARG:HB3	1.70	0.56
1:L:32:MET:SD	1:M:271:THR:HG21	2.45	0.56
1:P:78:GLU:O	1:P:82:VAL:HG23	2.05	0.56
1:B:231:ILE:HD12	1:B:263:LEU:HD13	1.87	0.56
1:J:105:GLU:HG3	1:K:228:GLU:HG2	1.87	0.56
1:R:9:LEU:HD13	1:R:11:PRO:HD3	1.87	0.56
1:E:323:ASN:HB2	1:E:367:MET:HG2	1.87	0.56
1:M:311:LEU:CD2	1:M:330:PRO:HG3	2.35	0.56
1:B:93:VAL:HG22	1:B:143:LEU:HB2	1.87	0.56
1:M:49:ASN:HD21	1:M:262:ARG:HH22	1.53	0.56
1:C:25:ASP:OD1	1:C:27:ARG:HD3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:OD1	1:A:176:THR:HG23	2.05	0.56
1:F:91:VAL:HG22	1:F:141:LEU:HB2	1.88	0.56
1:B:19:PRO:HD3	1:B:351:GLY:HA3	1.88	0.56
1:R:108:ARG:NH1	1:S:226:CYS:SG	2.79	0.56
1:G:105:GLU:HG3	1:H:228:GLU:HG2	1.88	0.56
1:O:105:GLU:HG3	1:P:229:GLU:H	1.71	0.55
1:G:25:ASP:OD1	1:G:27:ARG:HD3	2.06	0.55
1:G:33:SER:HB3	1:H:33:SER:HB3	1.86	0.55
1:K:126:THR:HG22	1:K:128:ASP:H	1.71	0.55
1:G:228:GLU:H	1:G:253:MET:HE3	1.71	0.55
1:D:299:GLY:O	1:D:303:VAL:HG23	2.06	0.55
1:H:25:ASP:OD1	1:H:27:ARG:HD3	2.06	0.55
1:O:141:LEU:HD13	1:O:170:LEU:HB2	1.87	0.55
1:K:295:HIS:CE1	1:K:368:GLY:H	2.21	0.55
1:H:82:VAL:HG12	1:H:244:ILE:HG23	1.88	0.55
1:B:27:ARG:HD2	1:D:10:ASN:ND2	2.22	0.55
1:P:299:GLY:O	1:P:303:VAL:HG23	2.07	0.55
1:L:199:GLN:HA	1:L:204:GLY:O	2.06	0.55
1:M:105:GLU:O	1:M:109:ARG:HG2	2.06	0.55
1:O:9:LEU:HD13	1:O:11:PRO:HD3	1.89	0.54
1:E:177:ALA:HA	1:E:200:LLP:HG3	1.90	0.54
1:O:271:THR:HG21	1:P:32:MET:SD	2.48	0.54
1:F:78:GLU:O	1:F:82:VAL:HG23	2.07	0.54
1:B:82:VAL:HG12	1:B:244:ILE:HG23	1.90	0.54
1:E:25:ASP:OD1	1:E:27:ARG:HD3	2.07	0.54
1:R:105:GLU:CG	1:S:229:GLU:H	2.19	0.54
1:K:49:ASN:HD21	1:K:262:ARG:HH22	1.55	0.54
1:R:390:LEU:O	1:R:391:LYS:CB	2.52	0.54
1:G:229:GLU:H	1:H:105:GLU:CG	2.21	0.54
1:H:141:LEU:HD13	1:H:170:LEU:HB2	1.90	0.54
1:S:299:GLY:O	1:S:303:VAL:HG23	2.08	0.53
1:E:341:LEU:O	1:E:345:ASP:HB2	2.08	0.53
1:J:33:SER:HB3	1:K:33:SER:HB3	1.90	0.53
1:S:323:ASN:HB2	1:S:367:MET:HG2	1.89	0.53
1:O:73:SER:HB3	1:O:176:THR:HG21	1.90	0.53
1:R:78:GLU:O	1:R:82:VAL:HG23	2.07	0.53
1:F:49:ASN:HD21	1:F:262:ARG:HH22	1.55	0.53
1:R:228:GLU:HG2	1:S:105:GLU:HG3	1.91	0.53
1:L:199:GLN:NE2	1:L:200:LLP:OP3	2.40	0.53
1:P:126:THR:HG22	1:P:128:ASP:H	1.72	0.53
1:H:82:VAL:HG12	1:H:244:ILE:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:149:THR:HA	1:J:321:MET:HE1	1.91	0.53
1:O:85:ILE:HG21	1:O:112:ALA:HB2	1.91	0.53
1:P:321:MET:SD	2:P:552:HOH:O	2.59	0.53
1:J:408:ARG:HB2	1:S:360:LYS:NZ	2.23	0.53
1:C:291:GLY:O	1:C:295:HIS:HD2	1.91	0.53
1:J:291:GLY:O	1:J:295:HIS:HD2	1.91	0.53
1:D:295:HIS:CE1	1:D:368:GLY:H	2.25	0.53
1:E:31:ALA:HB2	1:E:278:GLU:HG3	1.91	0.53
1:L:299:GLY:O	1:L:303:VAL:HG23	2.09	0.53
1:H:323:ASN:HB2	1:H:367:MET:HG2	1.91	0.53
1:G:177:ALA:HA	1:G:200:LLP:HG3	1.91	0.52
1:F:9:LEU:HD13	1:F:11:PRO:HD3	1.92	0.52
1:P:9:LEU:HD12	1:P:11:PRO:HD3	1.92	0.52
1:D:73:SER:HB3	1:D:176:THR:HG21	1.92	0.52
1:P:176:THR:HG22	1:P:196:ALA:C	2.30	0.52
1:B:84:ALA:O	1:B:140:ARG:NH1	2.43	0.52
1:F:83:SER:HA	1:F:244:ILE:HG12	1.91	0.52
1:R:295:HIS:HE1	1:R:368:GLY:N	2.08	0.52
1:J:405:ASP:O	1:S:360:LYS:HE3	2.10	0.52
1:M:79:ALA:HA	1:M:249:PHE:HB3	1.91	0.52
1:G:291:GLY:O	1:G:295:HIS:CD2	2.61	0.52
1:G:105:GLU:CG	1:H:229:GLU:H	2.22	0.52
1:J:105:GLU:CG	1:K:229:GLU:H	2.19	0.51
1:G:93:VAL:HG22	1:G:143:LEU:HB2	1.90	0.51
1:M:224:ARG:HD2	1:M:242:GLU:O	2.10	0.51
1:L:78:GLU:HG3	1:L:106:ILE:HG23	1.93	0.51
1:D:126:THR:HG22	1:D:128:ASP:H	1.74	0.51
1:C:94:PRO:HA	1:C:117:ILE:HG13	1.93	0.51
1:L:389:TYR:CZ	1:S:331:GLN:HB3	2.45	0.51
1:F:86:ARG:HH21	1:F:241:GLU:CD	2.13	0.51
1:C:9:LEU:HD23	1:D:277:ARG:HD3	1.92	0.51
1:S:153:MET:HE1	1:S:316:ASP:O	2.10	0.51
1:A:224:ARG:HD2	1:A:242:GLU:O	2.10	0.51
1:E:228:GLU:HG2	1:F:105:GLU:HG3	1.93	0.51
1:C:228:GLU:HG2	1:D:105:GLU:HG3	1.92	0.51
1:R:2:ASP:O	1:R:5:GLN:HG2	2.11	0.51
1:G:186:THR:HA	1:G:191:LEU:HD12	1.93	0.51
1:S:83:SER:HA	1:S:244:ILE:HG12	1.93	0.51
1:B:9:LEU:HD13	1:B:11:PRO:HD3	1.93	0.51
1:G:126:THR:H	1:G:129:GLN:NE2	2.07	0.51
1:B:24:ALA:HB1	2:B:833:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:135:LYS:HE3	1:K:167:TYR:OH	2.11	0.51
1:A:1:MET:HB3	1:A:2:ASP:HA	1.91	0.51
1:P:40:TYR:HE1	1:P:262:ARG:HB3	1.75	0.51
1:O:2:ASP:O	1:O:5:GLN:HG2	2.10	0.51
1:F:27:ARG:HD2	1:H:10:ASN:ND2	2.26	0.51
1:B:80:ILE:HD12	1:B:195:SER:HB3	1.93	0.50
1:B:47:TYR:O	1:B:51:VAL:HG23	2.11	0.50
1:L:105:GLU:HG3	1:M:229:GLU:H	1.75	0.50
1:L:146:GLN:NE2	1:L:178:SER:OG	2.44	0.50
1:H:73:SER:HB3	1:H:176:THR:HG21	1.93	0.50
1:D:91:VAL:HG22	1:D:141:LEU:HB2	1.94	0.50
1:J:49:ASN:HD21	1:J:262:ARG:HH22	1.60	0.50
1:K:73:SER:HB3	1:K:176:THR:HG21	1.92	0.50
1:C:141:LEU:HD13	1:C:170:LEU:HB2	1.93	0.50
1:H:348:ILE:HD11	1:H:378:THR:HG22	1.93	0.50
1:E:281:ARG:HH22	1:G:8:GLN:NE2	2.10	0.50
1:C:40:TYR:HE1	1:C:262:ARG:HB3	1.76	0.50
1:J:228:GLU:HB3	1:J:253:MET:HE1	1.94	0.50
1:L:126:THR:H	1:L:129:GLN:HE21	1.60	0.50
1:G:82:VAL:O	1:G:224:ARG:NH2	2.45	0.50
1:L:133:ALA:O	1:L:137:ILE:HD13	2.12	0.50
1:G:126:THR:H	1:G:129:GLN:HE21	1.59	0.49
1:D:92:LEU:HB2	1:D:137:ILE:HD11	1.94	0.49
1:C:32:MET:SD	1:D:271:THR:HG21	2.52	0.49
1:K:27:ARG:HD2	1:M:10:ASN:ND2	2.27	0.49
1:F:141:LEU:HD13	1:F:170:LEU:HB2	1.95	0.49
1:G:323:ASN:HB2	1:G:367:MET:HG2	1.94	0.49
1:C:72:THR:HG23	1:C:200:LLP:P	2.49	0.49
1:R:229:GLU:H	1:S:105:GLU:CG	2.23	0.49
1:A:228:GLU:HG2	1:B:105:GLU:HG3	1.93	0.49
1:D:9:LEU:CD1	1:D:11:PRO:HD3	2.43	0.49
1:S:303:VAL:HG22	1:S:325:LEU:HG	1.94	0.49
1:B:176:THR:HG22	1:B:196:ALA:HA	1.93	0.49
1:L:389:TYR:CE1	1:S:331:GLN:HB3	2.47	0.49
1:H:174:ASP:OD1	1:H:176:THR:HG23	2.12	0.49
1:L:141:LEU:HD13	1:L:170:LEU:HB2	1.94	0.49
1:G:265:HIS:HB2	2:G:440:HOH:O	2.10	0.49
1:R:224:ARG:HD2	1:R:242:GLU:O	2.13	0.49
1:C:82:VAL:O	1:C:224:ARG:NH2	2.46	0.49
1:E:33:SER:HB3	1:F:33:SER:HB3	1.95	0.49
1:M:329:ILE:HG12	1:M:362:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ALA:HB2	1:B:278:GLU:HG3	1.94	0.49
1:R:176:THR:HG22	1:R:196:ALA:HA	1.95	0.48
1:R:161:GLY:HA3	1:R:189:TRP:O	2.13	0.48
1:L:146:GLN:HG3	1:L:157:LEU:HD22	1.95	0.48
1:F:185:GLU:HB3	1:F:188:VAL:HB	1.94	0.48
1:J:19:PRO:HD3	1:J:351:GLY:HA3	1.94	0.48
1:A:126:THR:H	1:A:129:GLN:HE21	1.62	0.48
1:D:93:VAL:HG22	1:D:143:LEU:HB2	1.95	0.48
1:G:84:ALA:O	1:G:140:ARG:NH1	2.47	0.48
1:K:374:ASP:HA	1:M:345:ASP:O	2.13	0.48
1:D:121:TRP:HA	1:D:122:GLY:HA2	1.69	0.48
1:H:295:HIS:CE1	1:H:368:GLY:H	2.29	0.48
1:G:73:SER:HB3	1:G:176:THR:HG21	1.94	0.48
1:D:9:LEU:HD13	1:D:11:PRO:HD3	1.96	0.48
1:G:278:GLU:O	1:G:282:LEU:HG	2.13	0.48
1:J:78:GLU:O	1:J:82:VAL:HG23	2.14	0.48
1:F:85:ILE:O	1:F:224:ARG:NH2	2.47	0.48
1:L:3:ILE:HD13	1:M:284:LEU:HB2	1.94	0.48
1:F:152:THR:HA	1:F:321:MET:CE	2.43	0.48
1:R:181:GLY:HA2	1:R:295:HIS:CD2	2.49	0.48
1:F:152:THR:HA	1:F:321:MET:HE2	1.96	0.48
1:M:9:LEU:HD12	1:M:11:PRO:HD3	1.95	0.48
1:A:121:TRP:HA	1:A:122:GLY:HA2	1.71	0.48
1:F:52:MET:O	1:F:56:ARG:HG3	2.14	0.48
1:B:153:MET:HE1	1:B:316:ASP:HB3	1.95	0.48
1:G:79:ALA:HA	1:G:249:PHE:HB3	1.96	0.48
1:L:389:TYR:O	1:S:331:GLN:OE1	2.31	0.47
1:A:27:ARG:HD2	1:C:10:ASN:ND2	2.29	0.47
1:R:135:LYS:HE3	1:R:167:TYR:OH	2.14	0.47
1:H:19:PRO:HD3	1:H:351:GLY:HA3	1.96	0.47
1:E:78:GLU:O	1:E:82:VAL:HG23	2.14	0.47
1:J:331:GLN:HA	1:J:332:GLY:HA2	1.64	0.47
1:L:121:TRP:HA	1:L:122:GLY:HA2	1.71	0.47
1:H:94:PRO:HA	1:H:117:ILE:HG13	1.95	0.47
1:M:94:PRO:HA	1:M:117:ILE:HG13	1.96	0.47
1:C:74:ARG:HH21	1:C:102:LEU:HD13	1.79	0.47
1:J:229:GLU:H	1:K:105:GLU:CG	2.24	0.47
1:H:311:LEU:CD2	1:H:330:PRO:HG3	2.44	0.47
1:E:96:PHE:HB3	1:E:125:PHE:CE2	2.50	0.47
1:G:316:ASP:OD1	1:G:318:LYS:HE3	2.15	0.47
1:B:157:LEU:HG	1:B:171:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ASP:HA	1:F:214:SER:HB3	1.96	0.47
1:L:93:VAL:HG22	1:L:143:LEU:HB2	1.95	0.47
1:A:1:MET:HB3	1:A:2:ASP:CA	2.45	0.47
1:A:79:ALA:HA	1:A:249:PHE:HB3	1.97	0.47
1:P:177:ALA:HA	1:P:200:LLP:HG3	1.97	0.47
1:S:177:ALA:HA	1:S:200:LLP:HG3	1.97	0.47
1:A:78:GLU:O	1:A:82:VAL:HG23	2.15	0.47
1:P:205:PRO:HD2	2:P:903:HOH:O	2.14	0.47
1:B:299:GLY:O	1:B:303:VAL:HG23	2.14	0.47
1:P:192:ASP:HA	1:P:214:SER:HB3	1.96	0.47
1:C:79:ALA:HA	1:C:249:PHE:HB3	1.97	0.47
1:G:181:GLY:HA2	1:G:295:HIS:CD2	2.50	0.47
1:A:153:MET:HE1	1:A:319:HIS:HB2	1.95	0.47
1:C:227:VAL:HG21	1:C:236:HIS:CD2	2.49	0.47
1:L:295:HIS:CE1	1:L:368:GLY:H	2.32	0.47
1:G:66:THR:HG23	1:G:212:THR:HB	1.97	0.47
1:L:19:PRO:HD3	1:L:351:GLY:HA3	1.97	0.47
1:G:339:ARG:CZ	1:G:352:THR:HB	2.45	0.47
1:H:192:ASP:HB3	1:H:217:MET:HG2	1.97	0.47
1:C:49:ASN:HD21	1:C:262:ARG:HH22	1.63	0.47
1:H:299:GLY:O	1:H:303:VAL:HG23	2.16	0.47
1:D:254:VAL:O	1:D:258:TRP:HD1	1.98	0.46
1:O:105:GLU:CG	1:P:229:GLU:H	2.27	0.46
1:B:82:VAL:HG12	1:B:244:ILE:CG2	2.46	0.46
1:E:146:GLN:HE22	1:E:184:LEU:HD13	1.80	0.46
1:E:348:ILE:HD11	1:E:378:THR:HG22	1.96	0.46
1:C:105:GLU:HG3	1:D:228:GLU:HG2	1.96	0.46
1:B:224:ARG:HD2	1:B:242:GLU:O	2.16	0.46
1:J:80:ILE:HD12	1:J:195:SER:HB3	1.97	0.46
1:A:84:ALA:O	1:A:140:ARG:NH1	2.48	0.46
1:D:78:GLU:HG3	1:D:106:ILE:HG23	1.96	0.46
1:D:177:ALA:HB2	1:D:200:LLP:O3	2.16	0.46
1:D:82:VAL:O	1:D:224:ARG:NH2	2.49	0.46
1:B:28:VAL:HB	2:B:833:HOH:O	2.15	0.46
1:A:192:ASP:HB3	1:A:217:MET:HG2	1.97	0.46
1:S:121:TRP:HA	1:S:122:GLY:HA2	1.68	0.46
1:L:124:VAL:HG22	1:L:155:GLN:OE1	2.16	0.46
1:F:105:GLU:O	1:F:109:ARG:HG2	2.15	0.46
1:E:295:HIS:HE1	1:E:368:GLY:N	2.13	0.46
1:A:138:ARG:HH21	1:A:167:TYR:HB3	1.80	0.46
1:H:79:ALA:HA	1:H:249:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:TRP:HA	1:J:122:GLY:HA2	1.69	0.46
1:A:141:LEU:HD13	1:A:170:LEU:HB2	1.98	0.46
1:P:184:LEU:HD21	1:P:194:VAL:HG11	1.98	0.46
1:E:231:ILE:HD11	1:E:253:MET:HE3	1.97	0.46
1:G:74:ARG:HA	1:G:77:ILE:HD12	1.97	0.46
1:P:291:GLY:O	1:P:295:HIS:HD2	1.99	0.46
1:C:74:ARG:HA	1:C:77:ILE:HD12	1.97	0.46
1:A:329:ILE:HG12	1:A:362:TRP:CE2	2.50	0.46
1:G:121:TRP:HA	1:G:122:GLY:HA2	1.71	0.46
1:S:135:LYS:HE3	1:S:167:TYR:OH	2.16	0.46
1:H:91:VAL:HG22	1:H:141:LEU:HB2	1.97	0.45
1:A:199:GLN:HA	1:A:204:GLY:O	2.16	0.45
1:R:73:SER:HB3	1:R:176:THR:HG21	1.99	0.45
1:S:25:ASP:OD1	1:S:27:ARG:HD3	2.16	0.45
1:E:2:ASP:O	1:E:5:GLN:HG2	2.16	0.45
1:D:162:GLU:OE2	1:D:165:ARG:NH2	2.46	0.45
1:J:25:ASP:OD1	1:J:27:ARG:HD3	2.16	0.45
1:K:91:VAL:HG22	1:K:141:LEU:HB2	1.97	0.45
1:B:91:VAL:HG22	1:B:141:LEU:HB2	1.97	0.45
1:B:121:TRP:HA	1:B:122:GLY:HA2	1.72	0.45
1:P:295:HIS:HE1	1:P:368:GLY:N	2.08	0.45
1:K:299:GLY:O	1:K:303:VAL:HG23	2.16	0.45
1:G:299:GLY:O	1:G:303:VAL:HG23	2.16	0.45
1:M:219:GLU:O	1:M:223:ARG:HG3	2.16	0.45
1:P:329:ILE:HA	1:P:330:PRO:HD3	1.85	0.45
1:G:126:THR:HG22	1:G:128:ASP:H	1.81	0.45
1:L:3:ILE:HD13	1:M:284:LEU:CB	2.46	0.45
1:R:179:LEU:O	1:R:201:CYS:HB2	2.17	0.45
1:O:126:THR:HG22	1:O:128:ASP:H	1.82	0.45
1:J:224:ARG:HD2	1:J:242:GLU:O	2.17	0.45
1:R:98:ARG:NH1	1:R:102:LEU:HB2	2.31	0.45
1:M:231:ILE:HD11	1:M:253:MET:HE3	1.99	0.45
1:M:49:ASN:ND2	1:M:262:ARG:HH22	2.13	0.45
1:B:278:GLU:HG2	2:B:601:HOH:O	2.15	0.45
1:O:291:GLY:O	1:O:295:HIS:HD2	1.99	0.45
1:F:295:HIS:HE1	1:F:368:GLY:N	2.06	0.45
1:S:126:THR:HG22	1:S:128:ASP:H	1.82	0.45
1:A:105:GLU:O	1:A:109:ARG:HG2	2.17	0.45
1:D:152:THR:HA	1:D:321:MET:HE3	1.99	0.45
1:A:130:VAL:O	1:A:134:VAL:HG23	2.17	0.45
1:F:154:LEU:HD23	1:F:321:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:VAL:HG22	1:C:143:LEU:HB2	1.99	0.45
1:D:84:ALA:O	1:D:140:ARG:NH1	2.49	0.45
1:F:216:ARG:HG3	2:F:488:HOH:O	2.16	0.45
1:M:92:LEU:HB2	1:M:137:ILE:HD11	1.99	0.45
1:D:40:TYR:HE1	1:D:262:ARG:HB3	1.82	0.45
1:M:74:ARG:HA	1:M:77:ILE:HD12	1.99	0.44
1:A:5:GLN:H	1:A:5:GLN:HG2	1.59	0.44
1:H:74:ARG:HA	1:H:77:ILE:HD12	1.99	0.44
1:D:80:ILE:HD12	1:D:195:SER:HB3	1.99	0.44
1:E:93:VAL:HG22	1:E:143:LEU:HB2	2.00	0.44
1:B:141:LEU:HD13	1:B:170:LEU:HB2	1.98	0.44
1:P:48:MET:O	1:P:52:MET:HG3	2.16	0.44
1:H:82:VAL:O	1:H:224:ARG:NH2	2.51	0.44
1:D:203:GLY:N	1:D:204:GLY:HA3	2.32	0.44
1:F:30:ARG:HD2	1:G:30:ARG:O	2.17	0.44
1:S:146:GLN:NE2	1:S:178:SER:OG	2.50	0.44
1:F:10:ASN:ND2	1:H:27:ARG:HD2	2.33	0.44
1:R:121:TRP:HA	1:R:122:GLY:HA2	1.72	0.44
1:A:73:SER:HB3	1:A:176:THR:CG2	2.44	0.44
1:H:330:PRO:O	1:H:331:GLN:HB3	2.17	0.44
1:S:124:VAL:HG22	1:S:155:GLN:OE1	2.18	0.44
1:G:108:ARG:NH1	1:H:226:CYS:SG	2.90	0.44
1:D:146:GLN:NE2	1:D:178:SER:OG	2.51	0.44
1:R:61:THR:HB	1:R:186:THR:HB	2.00	0.44
1:A:229:GLU:H	1:B:105:GLU:CG	2.26	0.44
1:H:291:GLY:O	1:H:295:HIS:HD2	2.01	0.44
1:D:291:GLY:O	1:D:295:HIS:HD2	2.00	0.44
1:B:92:LEU:HD22	1:B:137:ILE:CD1	2.48	0.44
1:R:291:GLY:O	1:R:295:HIS:HD2	2.01	0.44
1:F:348:ILE:HD11	1:F:378:THR:HG22	2.00	0.44
1:O:135:LYS:HE2	1:O:167:TYR:OH	2.18	0.44
1:C:299:GLY:O	1:C:303:VAL:HG23	2.18	0.44
1:R:19:PRO:HD3	1:R:351:GLY:HA3	1.98	0.44
1:C:312:GLU:HG3	1:C:328:VAL:HB	2.00	0.43
1:B:69:VAL:HB	1:B:209:SER:HB3	1.99	0.43
1:F:36:LEU:HD22	1:F:270:THR:HB	2.00	0.43
1:A:19:PRO:HD3	1:A:351:GLY:HA3	2.01	0.43
1:O:19:PRO:HD3	1:O:351:GLY:HA3	1.99	0.43
1:E:31:ALA:CB	1:E:278:GLU:HG3	2.49	0.43
1:G:74:ARG:HD2	1:G:200:LLP:OP2	2.19	0.43
1:L:121:TRP:N	1:L:121:TRP:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:VAL:HB	1:F:116:THR:HG22	2.01	0.43
1:M:19:PRO:HD3	1:M:351:GLY:HA3	1.99	0.43
1:C:91:VAL:HG22	1:C:141:LEU:HB2	2.00	0.43
1:C:160:LEU:HA	1:C:163:ILE:HD12	2.00	0.43
1:O:10:ASN:ND2	1:R:27:ARG:HD2	2.34	0.43
1:O:27:ARG:HD2	1:R:10:ASN:ND2	2.33	0.43
1:C:149:THR:HG22	1:C:324:VAL:HG21	2.00	0.43
1:D:231:ILE:HD11	1:D:253:MET:CE	2.49	0.43
1:E:329:ILE:HG12	1:E:362:TRP:CE2	2.54	0.43
1:R:79:ALA:HA	1:R:249:PHE:HB3	2.01	0.43
1:M:80:ILE:HD12	1:M:195:SER:HB3	2.00	0.43
1:D:231:ILE:HD11	1:D:253:MET:HE3	2.00	0.43
1:K:85:ILE:O	1:K:224:ARG:NH2	2.52	0.43
1:S:253:MET:CE	1:S:265:HIS:HD2	2.32	0.43
1:J:92:LEU:HB2	1:J:137:ILE:HD11	2.01	0.43
1:J:146:GLN:NE2	1:J:184:LEU:HD13	2.34	0.43
1:M:299:GLY:O	1:M:303:VAL:HG23	2.19	0.43
1:E:345:ASP:O	1:G:374:ASP:HA	2.19	0.43
1:B:130:VAL:O	1:B:134:VAL:HG23	2.18	0.43
1:D:330:PRO:O	1:D:331:GLN:CB	2.67	0.43
1:D:161:GLY:HA3	1:D:189:TRP:O	2.18	0.43
1:O:27:ARG:NH2	1:O:282:LEU:HD22	2.33	0.43
1:E:329:ILE:HD13	1:E:335:GLY:HA3	2.01	0.43
1:H:295:HIS:HE1	1:H:368:GLY:N	2.14	0.42
1:S:141:LEU:HD13	1:S:170:LEU:HB2	2.00	0.42
1:P:219:GLU:O	1:P:223:ARG:HG3	2.19	0.42
1:R:149:THR:O	1:R:363:ARG:HD2	2.19	0.42
1:M:32:MET:HG2	1:M:271:THR:HG22	2.01	0.42
1:O:199:GLN:HA	1:O:204:GLY:O	2.19	0.42
1:B:146:GLN:NE2	1:B:178:SER:OG	2.52	0.42
1:J:179:LEU:O	1:J:201:CYS:HB2	2.19	0.42
1:A:341:LEU:O	1:A:345:ASP:HB2	2.18	0.42
1:F:121:TRP:HA	1:F:122:GLY:HA2	1.67	0.42
1:O:229:GLU:H	1:P:105:GLU:CG	2.27	0.42
1:P:52:MET:O	1:P:56:ARG:HG3	2.20	0.42
1:R:334:ASN:HB3	1:R:337:GLN:HB2	2.00	0.42
1:P:10:ASN:ND2	1:S:27:ARG:HD2	2.34	0.42
1:L:312:GLU:HB2	1:L:328:VAL:HB	2.01	0.42
1:S:74:ARG:HA	1:S:77:ILE:HD12	2.01	0.42
1:M:37:ILE:H	1:M:37:ILE:HD13	1.84	0.42
1:O:295:HIS:CE1	1:O:368:GLY:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:HIS:HE1	1:D:368:GLY:N	2.14	0.42
1:A:105:GLU:HG3	1:B:228:GLU:HG2	2.00	0.42
1:C:391:LYS:HB2	1:C:391:LYS:HE2	1.83	0.42
1:S:9:LEU:CD1	1:S:11:PRO:HD3	2.48	0.42
1:R:82:VAL:O	1:R:224:ARG:NH2	2.52	0.42
1:H:130:VAL:HG21	1:H:160:LEU:HG	2.02	0.42
1:M:135:LYS:HE3	1:M:167:TYR:OH	2.20	0.42
1:M:286:GLU:O	1:M:290:TYR:HD2	2.02	0.42
1:G:80:ILE:HD12	1:G:195:SER:HB3	2.00	0.42
1:E:19:PRO:HD3	1:E:351:GLY:HA3	2.01	0.42
1:G:226:CYS:SG	1:H:108:ARG:NH1	2.92	0.42
1:D:105:GLU:O	1:D:109:ARG:HG2	2.20	0.42
1:F:80:ILE:HD12	1:F:195:SER:HB3	2.01	0.42
1:H:121:TRP:HA	1:H:122:GLY:HA2	1.69	0.42
1:J:73:SER:HB2	1:J:200:LLP:OP4	2.20	0.42
1:C:73:SER:HB3	1:C:176:THR:HG21	2.01	0.42
1:C:105:GLU:CG	1:D:229:GLU:H	2.29	0.42
1:E:96:PHE:HB3	1:E:125:PHE:HE2	1.85	0.42
1:K:193:ALA:HB2	1:K:217:MET:HG3	2.02	0.42
1:A:121:TRP:CD1	1:A:121:TRP:N	2.86	0.42
1:J:320:LYS:HE2	1:J:324:VAL:O	2.20	0.42
1:E:339:ARG:NE	1:E:352:THR:HB	2.35	0.42
1:M:126:THR:H	1:M:129:GLN:NE2	2.10	0.41
1:L:105:GLU:O	1:L:109:ARG:HG3	2.20	0.41
1:B:9:LEU:CD1	1:B:11:PRO:HD3	2.50	0.41
1:A:2:ASP:CG	1:A:3:ILE:H	2.23	0.41
1:B:303:VAL:HG22	1:B:325:LEU:HG	2.01	0.41
1:F:179:LEU:O	1:F:201:CYS:HB2	2.20	0.41
1:K:79:ALA:HA	1:K:249:PHE:HB3	2.02	0.41
1:R:253:MET:HB3	1:R:253:MET:HE2	1.87	0.41
1:A:83:SER:C	1:A:224:ARG:HH21	2.24	0.41
1:O:300:ASP:HA	1:O:303:VAL:HG12	2.02	0.41
1:O:121:TRP:HA	1:O:122:GLY:HA2	1.70	0.41
1:E:98:ARG:NH1	1:E:102:LEU:HB2	2.35	0.41
1:J:48:MET:O	1:J:52:MET:HG3	2.21	0.41
1:L:85:ILE:O	1:L:224:ARG:NH2	2.53	0.41
1:P:152:THR:HA	1:P:321:MET:CE	2.50	0.41
1:C:78:GLU:O	1:C:82:VAL:HG23	2.19	0.41
1:C:82:VAL:HG12	1:C:244:ILE:HG23	2.03	0.41
1:D:52:MET:O	1:D:56:ARG:HG3	2.20	0.41
1:C:121:TRP:HA	1:C:122:GLY:HA2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:THR:H	1:J:129:GLN:NE2	2.19	0.41
1:J:91:VAL:HG22	1:J:141:LEU:HB2	2.02	0.41
1:F:203:GLY:HA2	2:F:586:HOH:O	2.19	0.41
1:C:224:ARG:HD2	1:C:242:GLU:O	2.21	0.41
1:F:149:THR:HA	1:F:321:MET:HE1	2.02	0.41
1:K:297:LEU:HD13	1:K:410:GLU:HG2	2.02	0.41
1:E:121:TRP:HA	1:E:122:GLY:HA2	1.68	0.41
1:C:19:PRO:HD3	1:C:351:GLY:HA3	2.02	0.41
1:F:295:HIS:CE1	1:F:368:GLY:N	2.85	0.41
1:P:218:GLU:HB3	2:P:523:HOH:O	2.21	0.41
1:S:198:MET:HB3	1:S:204:GLY:HA2	2.03	0.41
1:S:218:GLU:HG3	1:S:219:GLU:N	2.34	0.41
1:M:121:TRP:CD1	1:M:121:TRP:N	2.87	0.41
1:D:86:ARG:HB2	1:D:86:ARG:HE	1.69	0.41
1:E:146:GLN:NE2	1:E:184:LEU:HD13	2.36	0.41
1:H:133:ALA:O	1:H:137:ILE:HD13	2.21	0.41
1:R:348:ILE:HD11	1:R:378:THR:HG22	2.02	0.41
1:P:228:GLU:H	1:P:253:MET:HE1	1.85	0.41
1:L:389:TYR:CE2	1:S:331:GLN:HG2	2.55	0.41
1:J:82:VAL:HG12	1:J:244:ILE:HG23	2.02	0.41
1:A:149:THR:HA	1:A:321:MET:HE1	2.03	0.41
1:A:320:LYS:HE2	1:A:324:VAL:O	2.21	0.41
1:G:341:LEU:O	1:G:345:ASP:HB2	2.21	0.41
1:A:74:ARG:HA	1:A:77:ILE:HD12	2.03	0.41
1:P:121:TRP:HA	1:P:122:GLY:HA2	1.70	0.41
1:E:77:ILE:HG12	1:E:172:TYR:OH	2.21	0.41
1:B:74:ARG:HA	1:B:77:ILE:HD12	2.03	0.41
1:C:77:ILE:HG12	1:C:172:TYR:OH	2.21	0.41
1:J:133:ALA:O	1:J:137:ILE:HD13	2.21	0.41
1:M:327:VAL:HG21	1:M:364:ILE:HD12	2.03	0.41
1:C:329:ILE:HA	1:C:330:PRO:HD3	1.93	0.41
1:G:295:HIS:CE1	1:G:368:GLY:H	2.17	0.40
1:M:176:THR:HG22	1:M:196:ALA:CA	2.49	0.40
1:G:131:GLU:OE2	1:G:166:ARG:NH2	2.53	0.40
1:J:228:GLU:HG2	1:K:105:GLU:HG3	2.03	0.40
1:E:374:ASP:HA	1:G:345:ASP:O	2.21	0.40
1:S:291:GLY:O	1:S:295:HIS:HD2	2.04	0.40
1:L:21:PRO:HB3	1:L:199:GLN:HB2	2.03	0.40
1:B:78:GLU:O	1:B:82:VAL:HG23	2.21	0.40
1:O:224:ARG:HD2	1:O:242:GLU:O	2.21	0.40
1:M:179:LEU:O	1:M:201:CYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:278:GLU:O	1:S:282:LEU:HG	2.22	0.40
1:P:77:ILE:HG12	1:P:172:TYR:OH	2.21	0.40
1:S:92:LEU:HB2	1:S:137:ILE:HD11	2.02	0.40
1:K:9:LEU:CD1	1:K:11:PRO:HD3	2.37	0.40
1:H:105:GLU:O	1:H:109:ARG:HG2	2.22	0.40
1:F:176:THR:HG22	1:F:196:ALA:HA	2.02	0.40
1:R:355:GLY:HA3	1:R:356:PRO:HD2	1.84	0.40
1:D:2:ASP:O	1:D:5:GLN:HG2	2.21	0.40
1:J:5:GLN:HE21	1:J:5:GLN:HB3	1.72	0.40
1:L:91:VAL:HG22	1:L:141:LEU:HB2	2.03	0.40
1:D:199:GLN:HA	1:D:204:GLY:O	2.22	0.40
1:M:199:GLN:HA	1:M:204:GLY:O	2.21	0.40
1:C:22:ILE:HD11	2:C:619:HOH:O	2.22	0.40
1:G:133:ALA:O	1:G:137:ILE:HD13	2.21	0.40
1:A:92:LEU:HB2	1:A:137:ILE:HD11	2.02	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	408/411 (99%)	388 (95%)	20 (5%)	0	100	100
1	B	407/411 (99%)	390 (96%)	17 (4%)	0	100	100
1	C	407/411 (99%)	384 (94%)	22 (5%)	1 (0%)	52	75
1	D	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	52	75
1	E	407/411 (99%)	391 (96%)	15 (4%)	1 (0%)	52	75
1	F	407/411 (99%)	390 (96%)	17 (4%)	0	100	100
1	G	407/411 (99%)	391 (96%)	15 (4%)	1 (0%)	52	75
1	H	407/411 (99%)	395 (97%)	11 (3%)	1 (0%)	52	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	407/411 (99%)	392 (96%)	15 (4%)	0	100	100
1	K	407/411 (99%)	395 (97%)	12 (3%)	0	100	100
1	L	404/411 (98%)	391 (97%)	13 (3%)	0	100	100
1	M	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	52	75
1	O	407/411 (99%)	393 (97%)	14 (3%)	0	100	100
1	P	407/411 (99%)	392 (96%)	14 (3%)	1 (0%)	52	75
1	R	407/411 (99%)	395 (97%)	11 (3%)	1 (0%)	52	75
1	S	407/411 (99%)	394 (97%)	12 (3%)	1 (0%)	52	75
All	All	6510/6576 (99%)	6265 (96%)	236 (4%)	9 (0%)	56	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	331	GLN
1	R	391	LYS
1	D	331	GLN
1	G	226	CYS
1	S	246	SER
1	C	331	GLN
1	P	269	ALA
1	E	246	SER
1	M	203	GLY

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	323/336 (96%)	304 (94%)	19 (6%)	24	46
1	B	327/336 (97%)	308 (94%)	19 (6%)	25	47
1	C	324/336 (96%)	305 (94%)	19 (6%)	24	46
1	D	328/336 (98%)	312 (95%)	16 (5%)	31	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	321/336 (96%)	300 (94%)	21 (6%)	21 40
1	F	326/336 (97%)	312 (96%)	14 (4%)	35 62
1	G	324/336 (96%)	303 (94%)	21 (6%)	21 40
1	H	329/336 (98%)	310 (94%)	19 (6%)	25 47
1	J	323/336 (96%)	305 (94%)	18 (6%)	26 49
1	K	327/336 (97%)	313 (96%)	14 (4%)	35 62
1	L	323/336 (96%)	297 (92%)	26 (8%)	15 28
1	M	329/336 (98%)	312 (95%)	17 (5%)	29 53
1	O	323/336 (96%)	305 (94%)	18 (6%)	26 49
1	P	327/336 (97%)	308 (94%)	19 (6%)	25 47
1	R	324/336 (96%)	305 (94%)	19 (6%)	24 46
1	S	328/336 (98%)	307 (94%)	21 (6%)	22 42
All	All	5206/5376 (97%)	4906 (94%)	300 (6%)	25 47

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	LEU
1	A	22	ILE
1	A	34	SER
1	A	37	ILE
1	A	64	ARG
1	A	86	ARG
1	A	98	ARG
1	A	124	VAL
1	A	137	ILE
1	A	138	ARG
1	A	217	MET
1	A	222	ARG
1	A	324	VAL
1	A	325	LEU
1	A	377	MET
1	A	383	LEU
1	A	390	LEU
1	A	404	TRP
1	B	3	ILE
1	B	5	GLN

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Mol	Chain	Res	Type
1	B	9	LEU
1	B	37	ILE
1	B	86	ARG
1	B	98	ARG
1	B	124	VAL
1	B	137	ILE
1	B	165	ARG
1	B	168	ASP
1	B	217	MET
1	B	237	ARG
1	B	263	LEU
1	B	325	LEU
1	B	331	GLN
1	B	377	MET
1	B	383	LEU
1	B	404	TRP
1	B	410	GLU
1	C	9	LEU
1	C	22	ILE
1	C	37	ILE
1	C	72	THR
1	C	86	ARG
1	C	91	VAL
1	C	98	ARG
1	C	124	VAL
1	C	130	VAL
1	C	137	ILE
1	C	138	ARG
1	C	176	THR
1	C	217	MET
1	C	218	GLU
1	C	222	ARG
1	C	325	LEU
1	C	377	MET
1	C	383	LEU
1	C	404	TRP
1	D	9	LEU
1	D	37	ILE
1	D	86	ARG
1	D	98	ARG
1	D	124	VAL
1	D	137	ILE

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Mol	Chain	Res	Type
1	D	138	ARG
1	D	176	THR
1	D	217	MET
1	D	218	GLU
1	D	237	ARG
1	D	263	LEU
1	D	325	LEU
1	D	377	MET
1	D	383	LEU
1	D	404	TRP
1	E	9	LEU
1	E	22	ILE
1	E	37	ILE
1	E	86	ARG
1	E	91	VAL
1	E	98	ARG
1	E	124	VAL
1	E	137	ILE
1	E	138	ARG
1	E	154	LEU
1	E	176	THR
1	E	217	MET
1	E	218	GLU
1	E	224	ARG
1	E	237	ARG
1	E	273	LEU
1	E	325	LEU
1	E	377	MET
1	E	383	LEU
1	E	390	LEU
1	E	404	TRP
1	F	9	LEU
1	F	37	ILE
1	F	86	ARG
1	F	91	VAL
1	F	98	ARG
1	F	124	VAL
1	F	137	ILE
1	F	157	LEU
1	F	176	THR
1	F	237	ARG
1	F	325	LEU

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Mol	Chain	Res	Type
1	F	377	MET
1	F	383	LEU
1	F	404	TRP
1	G	9	LEU
1	G	22	ILE
1	G	37	ILE
1	G	86	ARG
1	G	91	VAL
1	G	98	ARG
1	G	124	VAL
1	G	137	ILE
1	G	138	ARG
1	G	176	THR
1	G	218	GLU
1	G	240	ASP
1	G	273	LEU
1	G	312	GLU
1	G	325	LEU
1	G	345	ASP
1	G	377	MET
1	G	383	LEU
1	G	390	LEU
1	G	391	LYS
1	G	404	TRP
1	H	4	THR
1	H	9	LEU
1	H	22	ILE
1	H	37	ILE
1	H	86	ARG
1	H	98	ARG
1	H	124	VAL
1	H	137	ILE
1	H	138	ARG
1	H	176	THR
1	H	217	MET
1	H	218	GLU
1	H	219	GLU
1	H	237	ARG
1	H	325	LEU
1	H	377	MET
1	H	383	LEU
1	H	390	LEU

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Mol	Chain	Res	Type
1	H	404	TRP
1	J	5	GLN
1	J	9	LEU
1	J	22	ILE
1	J	37	ILE
1	J	86	ARG
1	J	98	ARG
1	J	124	VAL
1	J	137	ILE
1	J	138	ARG
1	J	162	GLU
1	J	217	MET
1	J	218	GLU
1	J	222	ARG
1	J	324	VAL
1	J	325	LEU
1	J	377	MET
1	J	383	LEU
1	J	404	TRP
1	K	9	LEU
1	K	37	ILE
1	K	86	ARG
1	K	91	VAL
1	K	98	ARG
1	K	124	VAL
1	K	137	ILE
1	K	165	ARG
1	K	217	MET
1	K	222	ARG
1	K	324	VAL
1	K	325	LEU
1	K	383	LEU
1	K	404	TRP
1	L	9	LEU
1	L	22	ILE
1	L	27	ARG
1	L	37	ILE
1	L	60	ARG
1	L	74	ARG
1	L	82	VAL
1	L	86	ARG
1	L	91	VAL

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Mol	Chain	Res	Type
1	L	98	ARG
1	L	124	VAL
1	L	137	ILE
1	L	154	LEU
1	L	157	LEU
1	L	176	THR
1	L	217	MET
1	L	222	ARG
1	L	234	ASP
1	L	237	ARG
1	L	263	LEU
1	L	324	VAL
1	L	325	LEU
1	L	377	MET
1	L	383	LEU
1	L	390	LEU
1	L	404	TRP
1	M	4	THR
1	M	7	SER
1	M	9	LEU
1	M	37	ILE
1	M	86	ARG
1	M	98	ARG
1	M	124	VAL
1	M	126	THR
1	M	137	ILE
1	M	138	ARG
1	M	217	MET
1	M	218	GLU
1	M	325	LEU
1	M	377	MET
1	M	383	LEU
1	M	390	LEU
1	M	404	TRP
1	O	9	LEU
1	O	22	ILE
1	O	34	SER
1	O	37	ILE
1	O	86	ARG
1	O	91	VAL
1	O	98	ARG
1	O	124	VAL

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Mol	Chain	Res	Type
1	O	137	ILE
1	O	138	ARG
1	O	157	LEU
1	O	218	GLU
1	O	324	VAL
1	O	325	LEU
1	O	377	MET
1	O	383	LEU
1	O	390	LEU
1	O	404	TRP
1	P	9	LEU
1	P	22	ILE
1	P	37	ILE
1	P	86	ARG
1	P	91	VAL
1	P	98	ARG
1	P	108	ARG
1	P	124	VAL
1	P	137	ILE
1	P	138	ARG
1	P	165	ARG
1	P	217	MET
1	P	237	ARG
1	P	325	LEU
1	P	377	MET
1	P	383	LEU
1	P	390	LEU
1	P	391	LYS
1	P	404	TRP
1	R	9	LEU
1	R	22	ILE
1	R	37	ILE
1	R	60	ARG
1	R	74	ARG
1	R	86	ARG
1	R	98	ARG
1	R	124	VAL
1	R	130	VAL
1	R	137	ILE
1	R	138	ARG
1	R	165	ARG
1	R	217	MET

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Mol	Chain	Res	Type
1	R	222	ARG
1	R	325	LEU
1	R	377	MET
1	R	383	LEU
1	R	390	LEU
1	R	404	TRP
1	S	9	LEU
1	S	22	ILE
1	S	37	ILE
1	S	86	ARG
1	S	98	ARG
1	S	124	VAL
1	S	137	ILE
1	S	138	ARG
1	S	162	GLU
1	S	217	MET
1	S	218	GLU
1	S	222	ARG
1	S	237	ARG
1	S	263	LEU
1	S	325	LEU
1	S	336	ASP
1	S	377	MET
1	S	383	LEU
1	S	390	LEU
1	S	391	LYS
1	S	404	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	129	GLN
1	A	146	GLN
1	A	295	HIS
1	A	406	HIS
1	B	10	ASN
1	B	49	ASN
1	B	129	GLN
1	B	146	GLN
1	B	285	GLN

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Mol	Chain	Res	Type
1	B	295	HIS
1	B	331	GLN
1	C	8	GLN
1	C	10	ASN
1	C	39	GLN
1	C	49	ASN
1	C	129	GLN
1	C	146	GLN
1	C	295	HIS
1	C	406	HIS
1	D	5	GLN
1	D	10	ASN
1	D	39	GLN
1	D	49	ASN
1	D	129	GLN
1	D	146	GLN
1	D	295	HIS
1	D	406	HIS
1	E	5	GLN
1	E	10	ASN
1	E	49	ASN
1	E	101	HIS
1	E	129	GLN
1	E	146	GLN
1	E	295	HIS
1	E	406	HIS
1	F	10	ASN
1	F	49	ASN
1	F	129	GLN
1	F	146	GLN
1	F	295	HIS
1	F	388	ASN
1	G	5	GLN
1	G	8	GLN
1	G	10	ASN
1	G	39	GLN
1	G	46	HIS
1	G	49	ASN
1	G	129	GLN
1	G	146	GLN
1	G	295	HIS
1	G	406	HIS

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Mol	Chain	Res	Type
1	H	5	GLN
1	H	10	ASN
1	H	39	GLN
1	H	49	ASN
1	H	129	GLN
1	H	146	GLN
1	H	295	HIS
1	H	406	HIS
1	J	5	GLN
1	J	10	ASN
1	J	39	GLN
1	J	49	ASN
1	J	129	GLN
1	J	146	GLN
1	J	295	HIS
1	J	401	GLN
1	J	406	HIS
1	K	5	GLN
1	K	8	GLN
1	K	10	ASN
1	K	39	GLN
1	K	49	ASN
1	K	129	GLN
1	K	146	GLN
1	K	295	HIS
1	K	331	GLN
1	K	406	HIS
1	L	5	GLN
1	L	10	ASN
1	L	39	GLN
1	L	49	ASN
1	L	129	GLN
1	L	146	GLN
1	L	295	HIS
1	L	319	HIS
1	L	388	ASN
1	M	5	GLN
1	M	10	ASN
1	M	39	GLN
1	M	49	ASN
1	M	129	GLN
1	M	146	GLN

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Mol	Chain	Res	Type
1	M	295	HIS
1	M	388	ASN
1	M	406	HIS
1	O	5	GLN
1	O	10	ASN
1	O	39	GLN
1	O	49	ASN
1	O	129	GLN
1	O	146	GLN
1	O	295	HIS
1	O	388	ASN
1	O	406	HIS
1	P	5	GLN
1	P	10	ASN
1	P	39	GLN
1	P	49	ASN
1	P	129	GLN
1	P	146	GLN
1	P	295	HIS
1	P	406	HIS
1	R	5	GLN
1	R	10	ASN
1	R	39	GLN
1	R	49	ASN
1	R	129	GLN
1	R	146	GLN
1	R	295	HIS
1	S	5	GLN
1	S	10	ASN
1	S	39	GLN
1	S	49	ASN
1	S	129	GLN
1	S	146	GLN
1	S	295	HIS
1	S	331	GLN
1	S	406	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	A	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.56	5 (17%)
1	LLP	B	200	1	23,24,25	1.73	2 (8%)	28,32,34	1.88	7 (25%)
1	LLP	C	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.71	6 (21%)
1	LLP	D	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.70	5 (17%)
1	LLP	E	200	1	23,24,25	1.73	2 (8%)	28,32,34	1.82	6 (21%)
1	LLP	F	200	1	23,24,25	1.74	2 (8%)	28,32,34	1.64	5 (17%)
1	LLP	G	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.73	5 (17%)
1	LLP	H	200	1	23,24,25	1.74	2 (8%)	28,32,34	1.76	5 (17%)
1	LLP	J	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.59	5 (17%)
1	LLP	K	200	1	23,24,25	1.75	2 (8%)	28,32,34	1.86	5 (17%)
1	LLP	L	200	1	23,24,25	1.75	2 (8%)	28,32,34	1.59	5 (17%)
1	LLP	M	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.89	5 (17%)
1	LLP	O	200	1	23,24,25	1.72	2 (8%)	28,32,34	1.79	5 (17%)
1	LLP	P	200	1	23,24,25	1.74	2 (8%)	28,32,34	1.81	5 (17%)
1	LLP	R	200	1	23,24,25	1.74	2 (8%)	28,32,34	1.69	5 (17%)
1	LLP	S	200	1	23,24,25	1.76	2 (8%)	28,32,34	1.79	5 (17%)

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
1	LLP	A	200	1	-	1/15/17/19	0/1/1/1
1	LLP	B	200	1	-	0/15/17/19	0/1/1/1
1	LLP	C	200	1	-	0/15/17/19	0/1/1/1
1	LLP	D	200	1	-	0/15/17/19	0/1/1/1
1	LLP	E	200	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	F	200	1	-	0/15/17/19	0/1/1/1
1	LLP	G	200	1	-	0/15/17/19	0/1/1/1
1	LLP	H	200	1	-	0/15/17/19	0/1/1/1
1	LLP	J	200	1	-	1/15/17/19	0/1/1/1
1	LLP	K	200	1	-	0/15/17/19	0/1/1/1
1	LLP	L	200	1	-	1/15/17/19	0/1/1/1
1	LLP	M	200	1	-	0/15/17/19	0/1/1/1
1	LLP	O	200	1	-	0/15/17/19	0/1/1/1
1	LLP	P	200	1	-	0/15/17/19	0/1/1/1
1	LLP	R	200	1	-	0/15/17/19	0/1/1/1
1	LLP	S	200	1	-	1/15/17/19	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	LLP	C4-C4'	2.32	1.50	1.46
1	O	200	LLP	C4-C4'	2.34	1.50	1.46
1	M	200	LLP	C4-C4'	2.41	1.50	1.46
1	J	200	LLP	C4-C4'	2.44	1.50	1.46
1	E	200	LLP	C4-C4'	2.46	1.51	1.46
1	D	200	LLP	C4-C4'	2.48	1.51	1.46
1	R	200	LLP	C4-C4'	2.49	1.51	1.46
1	C	200	LLP	C4-C4'	2.49	1.51	1.46
1	P	200	LLP	C4-C4'	2.50	1.51	1.46
1	K	200	LLP	C4-C4'	2.50	1.51	1.46
1	H	200	LLP	C4-C4'	2.53	1.51	1.46
1	F	200	LLP	C4-C4'	2.55	1.51	1.46
1	L	200	LLP	C4-C4'	2.55	1.51	1.46
1	S	200	LLP	C4-C4'	2.59	1.51	1.46
1	A	200	LLP	C4-C4'	2.68	1.51	1.46
1	G	200	LLP	C4-C4'	2.69	1.51	1.46
1	E	200	LLP	C4'-NZ	7.04	1.48	1.27
1	O	200	LLP	C4'-NZ	7.06	1.48	1.27
1	B	200	LLP	C4'-NZ	7.07	1.48	1.27
1	R	200	LLP	C4'-NZ	7.08	1.48	1.27
1	C	200	LLP	C4'-NZ	7.08	1.48	1.27
1	P	200	LLP	C4'-NZ	7.09	1.48	1.27
1	M	200	LLP	C4'-NZ	7.10	1.48	1.27
1	H	200	LLP	C4'-NZ	7.11	1.48	1.27
1	L	200	LLP	C4'-NZ	7.13	1.48	1.27
1	A	200	LLP	C4'-NZ	7.15	1.48	1.27
1	D	200	LLP	C4'-NZ	7.17	1.48	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	200	LLP	C4'-NZ	7.17	1.48	1.27
1	J	200	LLP	C4'-NZ	7.17	1.48	1.27
1	S	200	LLP	C4'-NZ	7.18	1.48	1.27
1	F	200	LLP	C4'-NZ	7.18	1.48	1.27
1	G	200	LLP	C4'-NZ	7.19	1.49	1.27

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	200	LLP	CE-NZ-C4'	-3.54	108.74	118.97
1	O	200	LLP	CE-NZ-C4'	-3.48	108.91	118.97
1	F	200	LLP	CE-NZ-C4'	-3.44	109.02	118.97
1	S	200	LLP	CE-NZ-C4'	-3.39	109.17	118.97
1	P	200	LLP	CE-NZ-C4'	-3.35	109.31	118.97
1	E	200	LLP	CE-NZ-C4'	-3.33	109.36	118.97
1	C	200	LLP	CE-NZ-C4'	-3.29	109.47	118.97
1	J	200	LLP	CE-NZ-C4'	-3.28	109.50	118.97
1	R	200	LLP	CE-NZ-C4'	-3.28	109.51	118.97
1	D	200	LLP	CE-NZ-C4'	-3.26	109.55	118.97
1	A	200	LLP	CE-NZ-C4'	-3.23	109.63	118.97
1	K	200	LLP	CE-NZ-C4'	-3.22	109.68	118.97
1	M	200	LLP	CE-NZ-C4'	-3.20	109.74	118.97
1	G	200	LLP	CE-NZ-C4'	-3.17	109.82	118.97
1	L	200	LLP	CE-NZ-C4'	-3.00	110.29	118.97
1	B	200	LLP	CE-NZ-C4'	-2.70	111.17	118.97
1	M	200	LLP	O-C-CA	-2.66	118.55	125.49
1	R	200	LLP	O-C-CA	-2.63	118.65	125.49
1	B	200	LLP	O-C-CA	-2.62	118.66	125.49
1	M	200	LLP	C5-C6-N1	-2.59	119.37	123.86
1	B	200	LLP	C5-C6-N1	-2.56	119.42	123.86
1	A	200	LLP	O-C-CA	-2.56	118.83	125.49
1	K	200	LLP	O-C-CA	-2.56	118.83	125.49
1	S	200	LLP	O-C-CA	-2.54	118.86	125.49
1	P	200	LLP	C5-C6-N1	-2.51	119.50	123.86
1	L	200	LLP	O-C-CA	-2.51	118.95	125.49
1	D	200	LLP	O-C-CA	-2.51	118.95	125.49
1	G	200	LLP	O-C-CA	-2.51	118.96	125.49
1	E	200	LLP	C5-C6-N1	-2.49	119.54	123.86
1	H	200	LLP	C5-C6-N1	-2.48	119.55	123.86
1	C	200	LLP	C5-C6-N1	-2.47	119.57	123.86
1	E	200	LLP	O-C-CA	-2.47	119.06	125.49
1	H	200	LLP	O-C-CA	-2.46	119.08	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	200	LLP	O-C-CA	-2.46	119.09	125.49
1	O	200	LLP	C5-C6-N1	-2.43	119.64	123.86
1	K	200	LLP	C5-C6-N1	-2.41	119.68	123.86
1	J	200	LLP	O-C-CA	-2.38	119.30	125.49
1	J	200	LLP	C5-C6-N1	-2.37	119.75	123.86
1	S	200	LLP	C5-C6-N1	-2.36	119.77	123.86
1	R	200	LLP	C5-C6-N1	-2.35	119.79	123.86
1	G	200	LLP	C5-C6-N1	-2.33	119.82	123.86
1	F	200	LLP	O-C-CA	-2.32	119.44	125.49
1	F	200	LLP	C5-C6-N1	-2.31	119.85	123.86
1	L	200	LLP	C5-C6-N1	-2.29	119.88	123.86
1	O	200	LLP	O-C-CA	-2.26	119.61	125.49
1	D	200	LLP	C5-C6-N1	-2.24	119.97	123.86
1	P	200	LLP	O-C-CA	-2.24	119.67	125.49
1	A	200	LLP	C5-C6-N1	-2.19	120.06	123.86
1	B	200	LLP	C4-C4'-NZ	-2.04	113.69	125.06
1	E	200	LLP	O3-C3-C2	2.01	121.16	117.66
1	C	200	LLP	OP3-P-OP4	2.02	112.37	106.56
1	B	200	LLP	O3-C3-C2	2.07	121.27	117.66
1	C	200	LLP	CD-CE-NZ	3.29	116.36	110.98
1	E	200	LLP	CD-CE-NZ	3.30	116.38	110.98
1	L	200	LLP	CD-CE-NZ	3.37	116.49	110.98
1	B	200	LLP	CD-CE-NZ	3.50	116.71	110.98
1	H	200	LLP	CD-CE-NZ	3.52	116.74	110.98
1	R	200	LLP	CD-CE-NZ	3.53	116.75	110.98
1	D	200	LLP	CD-CE-NZ	3.59	116.86	110.98
1	G	200	LLP	CD-CE-NZ	3.77	117.16	110.98
1	P	200	LLP	CD-CE-NZ	3.79	117.19	110.98
1	J	200	LLP	CD-CE-NZ	3.86	117.29	110.98
1	A	200	LLP	CD-CE-NZ	3.86	117.31	110.98
1	F	200	LLP	CD-CE-NZ	3.88	117.33	110.98
1	K	200	LLP	CD-CE-NZ	4.02	117.56	110.98
1	A	200	LLP	OP4-C5'-C5	4.05	115.69	108.99
1	O	200	LLP	CD-CE-NZ	4.08	117.66	110.98
1	S	200	LLP	CD-CE-NZ	4.09	117.67	110.98
1	J	200	LLP	OP4-C5'-C5	4.36	116.20	108.99
1	M	200	LLP	CD-CE-NZ	4.48	118.31	110.98
1	F	200	LLP	OP4-C5'-C5	4.78	116.89	108.99
1	L	200	LLP	OP4-C5'-C5	4.90	117.10	108.99
1	R	200	LLP	OP4-C5'-C5	5.16	117.52	108.99
1	C	200	LLP	OP4-C5'-C5	5.36	117.85	108.99
1	D	200	LLP	OP4-C5'-C5	5.48	118.05	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	200	LLP	OP4-C5'-C5	5.62	118.29	108.99
1	O	200	LLP	OP4-C5'-C5	5.64	118.32	108.99
1	S	200	LLP	OP4-C5'-C5	5.78	118.54	108.99
1	H	200	LLP	OP4-C5'-C5	5.80	118.58	108.99
1	P	200	LLP	OP4-C5'-C5	6.04	118.98	108.99
1	M	200	LLP	OP4-C5'-C5	6.10	119.07	108.99
1	E	200	LLP	OP4-C5'-C5	6.32	119.44	108.99
1	K	200	LLP	OP4-C5'-C5	6.43	119.62	108.99
1	B	200	LLP	OP4-C5'-C5	6.60	119.90	108.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	200	LLP	C4-C4'-NZ-CE
1	A	200	LLP	C4-C4'-NZ-CE
1	L	200	LLP	C4-C4'-NZ-CE
1	S	200	LLP	C4-C4'-NZ-CE

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	200	LLP	3	0
1	D	200	LLP	2	0
1	E	200	LLP	1	0
1	G	200	LLP	2	0
1	J	200	LLP	1	0
1	L	200	LLP	2	0
1	P	200	LLP	1	0
1	R	200	LLP	1	0
1	S	200	LLP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	410/411 (99%)	0.74	46 (11%) 7 5	26, 36, 45, 53	0
1	B	409/411 (99%)	0.77	40 (9%) 10 7	27, 33, 43, 57	0
1	C	409/411 (99%)	0.72	31 (7%) 17 13	26, 34, 47, 57	0
1	D	409/411 (99%)	0.49	14 (3%) 49 43	26, 33, 42, 46	0
1	E	409/411 (99%)	0.58	24 (5%) 26 21	25, 35, 44, 48	0
1	F	409/411 (99%)	0.53	25 (6%) 25 20	26, 32, 43, 56	0
1	G	409/411 (99%)	0.81	40 (9%) 10 7	26, 34, 45, 58	0
1	H	409/411 (99%)	0.49	22 (5%) 29 24	25, 32, 41, 47	0
1	J	409/411 (99%)	0.52	19 (4%) 36 31	25, 31, 41, 46	0
1	K	409/411 (99%)	0.79	37 (9%) 12 9	25, 31, 44, 55	0
1	L	408/411 (99%)	0.49	27 (6%) 22 17	25, 32, 43, 61	0
1	M	409/411 (99%)	0.49	18 (4%) 38 33	25, 33, 42, 46	0
1	O	409/411 (99%)	0.35	9 (2%) 65 61	24, 31, 41, 46	0
1	P	409/411 (99%)	0.51	19 (4%) 36 31	25, 32, 44, 55	0
1	R	409/411 (99%)	0.80	38 (9%) 11 8	27, 32, 43, 61	0
1	S	409/411 (99%)	0.58	24 (5%) 26 21	27, 33, 43, 46	0
All	All	6544/6576 (99%)	0.60	433 (6%) 22 17	24, 33, 44, 61	0

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	233	THR	9.3
1	L	235	ALA	8.3
1	R	234	ASP	8.1
1	B	235	ALA	6.8
1	R	227	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	234	ASP	6.8
1	R	237	ARG	6.3
1	K	237	ARG	6.3
1	R	226	CYS	6.1
1	K	234	ASP	5.7
1	R	235	ALA	5.4
1	B	237	ARG	5.3
1	A	137	ILE	5.2
1	G	237	ARG	5.2
1	A	359	GLY	5.1
1	B	233	THR	5.0
1	O	137	ILE	4.9
1	R	308	ALA	4.8
1	J	290	TYR	4.7
1	C	235	ALA	4.7
1	K	235	ALA	4.6
1	C	227	VAL	4.6
1	L	227	VAL	4.6
1	S	133	ALA	4.6
1	K	2	ASP	4.5
1	A	130	VAL	4.5
1	H	165	ARG	4.5
1	L	229	GLU	4.4
1	G	234	ASP	4.4
1	H	335	GLY	4.4
1	A	129	GLN	4.4
1	R	160	LEU	4.4
1	R	231	ILE	4.4
1	G	390	LEU	4.4
1	R	232	ARG	4.4
1	J	354	PHE	4.4
1	C	232	ARG	4.3
1	A	91	VAL	4.3
1	B	390	LEU	4.3
1	C	233	THR	4.3
1	J	333	ILE	4.3
1	B	188	VAL	4.3
1	K	230	GLY	4.3
1	S	137	ILE	4.2
1	B	232	ARG	4.2
1	K	188	VAL	4.2
1	A	119	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	233	THR	4.1
1	G	227	VAL	4.0
1	K	233	THR	4.0
1	R	228	GLU	4.0
1	C	4	THR	4.0
1	C	162	GLU	3.9
1	F	228	GLU	3.9
1	D	137	ILE	3.9
1	M	292	ILE	3.9
1	K	232	ARG	3.8
1	C	326	GLY	3.8
1	R	354	PHE	3.8
1	B	231	ILE	3.7
1	E	328	VAL	3.7
1	P	359	GLY	3.7
1	A	167	TYR	3.6
1	G	31	ALA	3.6
1	C	144	THR	3.6
1	S	138	ARG	3.6
1	C	57	GLY	3.6
1	G	411	ARG	3.6
1	K	238	ASP	3.6
1	L	167	TYR	3.5
1	B	329	ILE	3.5
1	J	334	ASN	3.5
1	L	234	ASP	3.5
1	P	238	ASP	3.5
1	B	205	PRO	3.5
1	F	29	LEU	3.5
1	R	184	LEU	3.5
1	A	354	PHE	3.5
1	E	354	PHE	3.5
1	E	290	TYR	3.4
1	H	137	ILE	3.4
1	R	236	HIS	3.4
1	R	133	ALA	3.4
1	H	290	TYR	3.4
1	L	236	HIS	3.4
1	P	308	ALA	3.4
1	G	232	ARG	3.4
1	G	231	ILE	3.4
1	A	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	334	ASN	3.3
1	A	5	GLN	3.3
1	L	333	ILE	3.3
1	A	314	PHE	3.3
1	C	353	SER	3.3
1	E	219	GLU	3.3
1	A	191	LEU	3.3
1	G	351	GLY	3.3
1	P	188	VAL	3.2
1	A	158	ALA	3.2
1	B	360	LYS	3.2
1	B	289	ASP	3.2
1	C	316	ASP	3.2
1	E	128	ASP	3.2
1	C	5	GLN	3.2
1	K	229	GLU	3.2
1	R	164	CYS	3.1
1	K	290	TYR	3.1
1	C	315	GLY	3.1
1	A	132	ASP	3.1
1	B	290	TYR	3.1
1	P	36	LEU	3.1
1	J	34	SER	3.1
1	S	130	VAL	3.1
1	B	166	ARG	3.1
1	K	228	GLU	3.0
1	G	233	THR	3.0
1	G	395	THR	3.0
1	A	163	ILE	3.0
1	F	231	ILE	3.0
1	B	303	VAL	3.0
1	P	227	VAL	3.0
1	R	305	GLY	3.0
1	J	271	THR	3.0
1	A	124	VAL	3.0
1	G	356	PRO	3.0
1	R	316	ASP	3.0
1	G	271	THR	3.0
1	B	359	GLY	3.0
1	J	360	LYS	3.0
1	L	290	TYR	3.0
1	A	164	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	120	PRO	2.9
1	K	273	LEU	2.9
1	H	162	GLU	2.9
1	F	312	GLU	2.9
1	H	390	LEU	2.9
1	B	236	HIS	2.9
1	L	237	ARG	2.9
1	C	124	VAL	2.9
1	M	2	ASP	2.9
1	M	188	VAL	2.9
1	E	409	SER	2.9
1	J	359	GLY	2.9
1	H	33	SER	2.9
1	A	134	VAL	2.9
1	R	159	GLU	2.9
1	A	358	HIS	2.9
1	D	126	THR	2.9
1	F	137	ILE	2.9
1	H	354	PHE	2.8
1	F	232	ARG	2.8
1	A	352	THR	2.8
1	M	168	ASP	2.8
1	A	355	GLY	2.8
1	C	229	GLU	2.8
1	D	132	ASP	2.8
1	A	4	THR	2.8
1	G	235	ALA	2.8
1	R	137	ILE	2.8
1	F	236	HIS	2.8
1	S	165	ARG	2.8
1	G	361	VAL	2.8
1	L	134	VAL	2.8
1	R	239	GLY	2.8
1	C	165	ARG	2.8
1	O	138	ARG	2.8
1	K	106	ILE	2.8
1	S	187	ASP	2.8
1	A	136	ARG	2.8
1	M	360	LYS	2.8
1	J	137	ILE	2.7
1	D	28	VAL	2.7
1	G	303	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	4	THR	2.7
1	A	33	SER	2.7
1	G	391	LYS	2.7
1	B	356	PRO	2.7
1	S	158	ALA	2.7
1	P	166	ARG	2.7
1	S	2	ASP	2.7
1	G	354	PHE	2.7
1	L	232	ARG	2.7
1	K	29	LEU	2.7
1	G	270	THR	2.7
1	L	4	THR	2.7
1	C	320	LYS	2.7
1	H	168	ASP	2.7
1	G	263	LEU	2.7
1	J	29	LEU	2.7
1	B	124	VAL	2.7
1	O	354	PHE	2.7
1	M	136	ARG	2.6
1	B	29	LEU	2.6
1	G	236	HIS	2.6
1	S	36	LEU	2.6
1	J	2	ASP	2.6
1	J	240	ASP	2.6
1	A	162	GLU	2.6
1	R	166	ARG	2.6
1	A	356	PRO	2.6
1	G	383	LEU	2.6
1	H	31	ALA	2.6
1	K	392	PHE	2.6
1	J	361	VAL	2.6
1	L	228	GLU	2.6
1	L	239	GLY	2.6
1	F	334	ASN	2.6
1	B	331	GLN	2.6
1	M	130	VAL	2.6
1	D	335	GLY	2.6
1	E	167	TYR	2.6
1	G	29	LEU	2.6
1	A	121	TRP	2.6
1	B	226	CYS	2.6
1	J	358	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	392	PHE	2.6
1	O	33	SER	2.5
1	F	393	PRO	2.5
1	G	167	TYR	2.5
1	P	360	LYS	2.5
1	H	169	ALA	2.5
1	R	128	ASP	2.5
1	B	354	PHE	2.5
1	G	162	GLU	2.5
1	S	287	GLY	2.5
1	L	226	CYS	2.5
1	E	4	THR	2.5
1	C	234	ASP	2.5
1	K	6	PHE	2.5
1	S	204	GLY	2.5
1	J	33	SER	2.5
1	L	34	SER	2.5
1	D	5	GLN	2.5
1	J	327	VAL	2.5
1	A	390	LEU	2.5
1	O	92	LEU	2.5
1	A	133	ALA	2.5
1	K	272	ALA	2.5
1	S	31	ALA	2.5
1	R	168	ASP	2.5
1	S	360	LYS	2.5
1	M	137	ILE	2.5
1	R	163	ILE	2.5
1	M	34	SER	2.5
1	K	354	PHE	2.4
1	A	2	ASP	2.4
1	B	330	PRO	2.4
1	D	236	HIS	2.4
1	D	165	ARG	2.4
1	D	391	LYS	2.4
1	R	132	ASP	2.4
1	S	162	GLU	2.4
1	E	327	VAL	2.4
1	E	186	THR	2.4
1	A	353	SER	2.4
1	P	353	SER	2.4
1	B	60	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	167	TYR	2.4
1	D	138	ARG	2.4
1	R	136	ARG	2.4
1	J	5	GLN	2.4
1	S	290	TYR	2.4
1	K	205	PRO	2.4
1	K	236	HIS	2.4
1	K	386	VAL	2.4
1	O	28	VAL	2.4
1	G	313	THR	2.4
1	S	3	ILE	2.4
1	R	5	GLN	2.4
1	R	32	MET	2.4
1	G	328	VAL	2.4
1	F	352	THR	2.4
1	K	271	THR	2.4
1	H	163	ILE	2.4
1	E	398	ALA	2.4
1	F	167	TYR	2.4
1	F	392	PHE	2.4
1	H	167	TYR	2.4
1	P	237	ARG	2.4
1	S	33	SER	2.3
1	A	364	ILE	2.3
1	F	333	ILE	2.3
1	C	334	ASN	2.3
1	R	393	PRO	2.3
1	L	238	ASP	2.3
1	C	130	VAL	2.3
1	K	126	THR	2.3
1	L	360	LYS	2.3
1	M	333	ILE	2.3
1	P	231	ILE	2.3
1	A	240	ASP	2.3
1	S	119	VAL	2.3
1	R	332	GLY	2.3
1	G	133	ALA	2.3
1	G	219	GLU	2.3
1	M	22	ILE	2.3
1	K	302	LEU	2.3
1	P	290	TYR	2.3
1	E	385	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	356	PRO	2.3
1	C	228	GLU	2.3
1	A	126	THR	2.3
1	B	32	MET	2.3
1	E	306	ILE	2.3
1	R	229	GLU	2.3
1	O	34	SER	2.3
1	D	390	LEU	2.3
1	E	121	TRP	2.3
1	F	330	PRO	2.3
1	A	96	PHE	2.2
1	M	246	SER	2.2
1	K	387	LEU	2.2
1	F	290	TYR	2.2
1	G	26	PRO	2.2
1	B	75	ALA	2.2
1	F	53	ALA	2.2
1	G	22	ILE	2.2
1	C	237	ARG	2.2
1	L	5	GLN	2.2
1	G	32	MET	2.2
1	B	128	ASP	2.2
1	S	240	ASP	2.2
1	K	203	GLY	2.2
1	K	314	PHE	2.2
1	L	355	GLY	2.2
1	E	384	GLU	2.2
1	H	234	ASP	2.2
1	P	37	ILE	2.2
1	A	122	GLY	2.2
1	A	154	LEU	2.2
1	B	36	LEU	2.2
1	E	36	LEU	2.2
1	K	263	LEU	2.2
1	K	331	GLN	2.2
1	L	378	THR	2.2
1	R	290	TYR	2.2
1	B	308	ALA	2.2
1	L	385	ALA	2.2
1	P	64	ARG	2.2
1	B	273	LEU	2.2
1	E	134	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	2.2
1	C	383	LEU	2.2
1	P	29	LEU	2.2
1	M	313	THR	2.2
1	C	238	ASP	2.2
1	B	206	SER	2.1
1	B	389	TYR	2.1
1	F	403	ALA	2.1
1	G	230	GLY	2.1
1	R	201	CYS	2.1
1	A	128	ASP	2.1
1	R	9	LEU	2.1
1	C	362	TRP	2.1
1	A	327	VAL	2.1
1	E	133	ALA	2.1
1	F	206	SER	2.1
1	H	305	GLY	2.1
1	S	35	GLN	2.1
1	F	215	ALA	2.1
1	F	32	MET	2.1
1	B	106	ILE	2.1
1	H	138	ARG	2.1
1	B	271	THR	2.1
1	D	121	TRP	2.1
1	G	130	VAL	2.1
1	S	114	VAL	2.1
1	J	162	GLU	2.1
1	R	162	GLU	2.1
1	B	96	PHE	2.1
1	K	279	CYS	2.1
1	J	24	ALA	2.1
1	R	134	VAL	2.1
1	M	312	GLU	2.1
1	R	118	GLU	2.1
1	H	3	ILE	2.1
1	G	273	LEU	2.1
1	G	314	PHE	2.1
1	H	311	LEU	2.1
1	C	270	THR	2.1
1	C	335	GLY	2.1
1	C	358	HIS	2.1
1	G	205	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	178	SER	2.1
1	B	361	VAL	2.1
1	H	336	ASP	2.1
1	M	121	TRP	2.1
1	S	189	TRP	2.1
1	H	36	LEU	2.1
1	M	205	PRO	2.1
1	E	162	GLU	2.1
1	F	353	SER	2.1
1	M	402	ALA	2.1
1	D	167	TYR	2.1
1	L	359	GLY	2.1
1	P	275	GLY	2.1
1	E	141	LEU	2.1
1	G	240	ASP	2.1
1	A	123	GLU	2.0
1	L	130	VAL	2.0
1	S	188	VAL	2.0
1	K	71	GLY	2.0
1	M	26	PRO	2.0
1	P	9	LEU	2.0
1	S	4	THR	2.0
1	B	165	ARG	2.0
1	F	216	ARG	2.0
1	L	165	ARG	2.0
1	B	358	HIS	2.0
1	E	364	ILE	2.0
1	K	260	PRO	2.0
1	O	2	ASP	2.0
1	A	116	THR	2.0
1	B	392	PHE	2.0
1	D	186	THR	2.0
1	G	176	THR	2.0
1	G	274	PHE	2.0
1	K	4	THR	2.0
1	K	176	THR	2.0
1	L	354	PHE	2.0
1	C	223	ARG	2.0
1	F	31	ALA	2.0
1	E	124	VAL	2.0
1	E	188	VAL	2.0
1	E	303	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	230	GLY	2.0
1	A	3	ILE	2.0
1	A	329	ILE	2.0
1	K	289	ASP	2.0
1	O	333	ILE	2.0
1	K	36	LEU	2.0
1	C	290	TYR	2.0
1	F	270	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	LLP	R	200	24/25	0.94	0.20	-	29,31,31,32	0
1	LLP	S	200	24/25	0.93	0.19	-	31,32,33,33	0
1	LLP	E	200	24/25	0.94	0.16	-	31,32,33,33	0
1	LLP	F	200	24/25	0.96	0.15	-	28,30,30,31	0
1	LLP	G	200	24/25	0.93	0.22	-	30,31,31,31	0
1	LLP	H	200	24/25	0.94	0.18	-	28,31,32,33	0
1	LLP	A	200	24/25	0.91	0.19	-	32,33,35,35	0
1	LLP	B	200	24/25	0.93	0.19	-	29,30,32,32	0
1	LLP	C	200	24/25	0.93	0.17	-	32,33,33,34	0
1	LLP	D	200	24/25	0.93	0.20	-	29,30,30,31	0
1	LLP	M	200	24/25	0.93	0.18	-	30,33,34,35	0
1	LLP	O	200	24/25	0.94	0.18	-	28,30,31,31	0
1	LLP	P	200	24/25	0.95	0.15	-	30,32,32,32	0
1	LLP	J	200	24/25	0.96	0.18	-	28,30,30,30	0
1	LLP	K	200	24/25	0.94	0.20	-	29,31,31,32	0
1	LLP	L	200	24/25	0.94	0.19	-	28,29,30,30	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.