Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:20 PM GMT

PDB ID	:	3TMK
Title	:	CRYSTAL STRUCTURE OF YEAST THYMIDYLATE KINASE COMPLEXED WITH THE BISUBSTRATE INHIBITOR TP5A AT 2.0 A RESOLUTION: IMPLICATIONS FOR CATALYSIS AND AZT ACTIVATION
Authors	:	Lavie, A.; Schlichting, I.; Konrad, M.; Goody, R.S.; Brundiers, R.; Reinstein, J.
Deposited on	:	1998-01-26
Resolution	:	2.00 Å(reported)

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

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

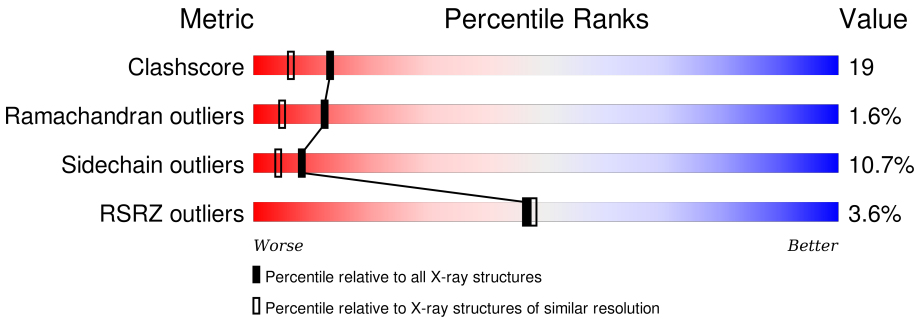
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	6% 58% 34% 7%
1	B	216	2% 72% 25% •
1	C	216	2% 52% 32% 11% 5%
1	D	216	2% 70% 25% • •
1	E	216	6% 61% 33% 5%
1	F	216	2% 70% 25% •
1	G	216	4% 61% 30% 8%

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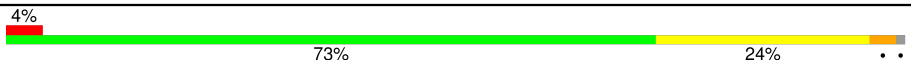
Mol	Chain	Length	Quality of chain
1	H	216	

2 Entry composition (i)

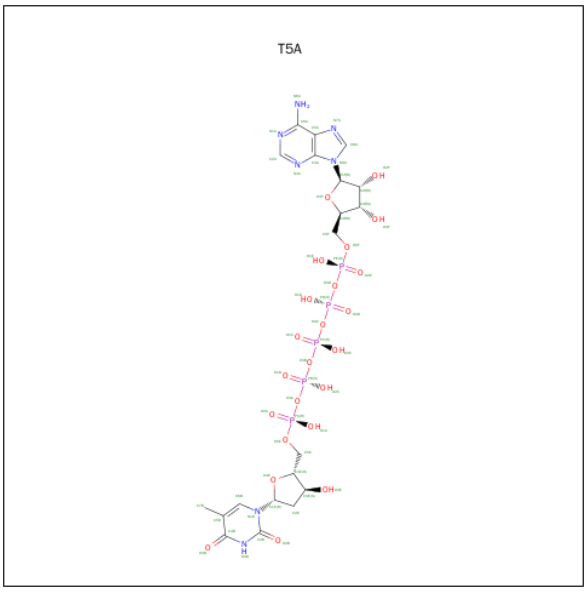
There are 3 unique types of molecules in this entry. The entry contains 15240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1107	289	332	8			
1	B	216	Total	C	N	O	S	0	0	0
			1733	1106	289	330	8			
1	C	205	Total	C	N	O	S	0	0	0
			1657	1060	275	314	8			
1	D	214	Total	C	N	O	S	0	0	0
			1707	1092	286	323	6			
1	E	215	Total	C	N	O	S	0	0	0
			1722	1096	288	331	7			
1	F	216	Total	C	N	O	S	0	0	0
			1729	1104	288	329	8			
1	G	215	Total	C	N	O	S	0	0	0
			1722	1096	288	331	7			
1	H	214	Total	C	N	O	S	0	0	0
			1706	1090	285	325	6			

- Molecule 2 is P1-(5'-ADENOSYL)P5-(5'-THYMIDYL)PENTAPHOSPHATE (three-letter code: T5A) (formula: $C_{20}H_{30}N_7O_{23}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	B	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	C	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	D	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	E	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	F	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	G	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	H	1	Total	C	N	O	P	0	0
			55	20	7	23	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	161	Total	O	0	0
			161	161		
3	C	134	Total	O	0	0
			134	134		
3	D	144	Total	O	0	0
			144	144		

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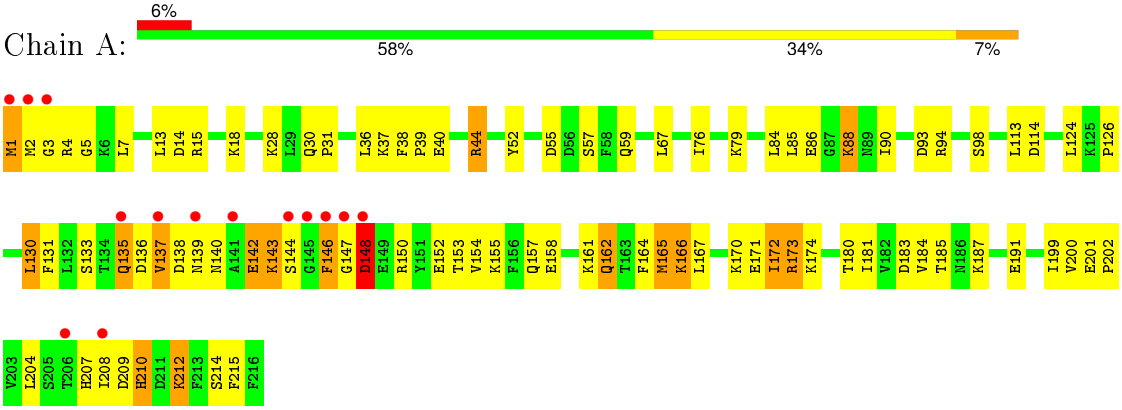
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	126	Total O 126 126	0	0
3	F	147	Total O 147 147	0	0
3	G	136	Total O 136 136	0	0
3	H	111	Total O 111 111	0	0

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.

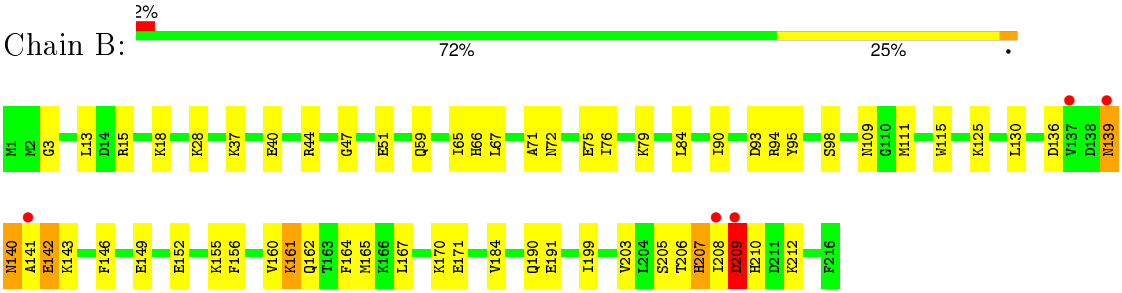
- Molecule 1: THYMIDYLATE KINASE

Chain A:



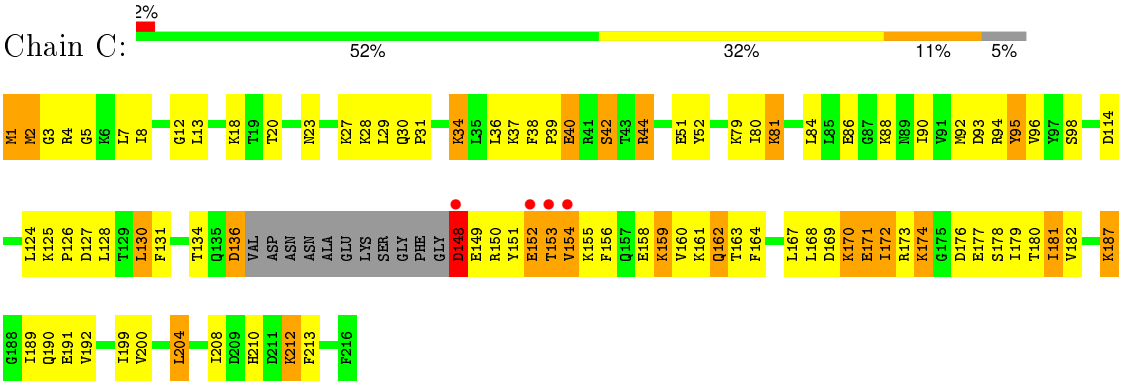
- Molecule 1: THYMIDYLATE KINASE

Chain B:



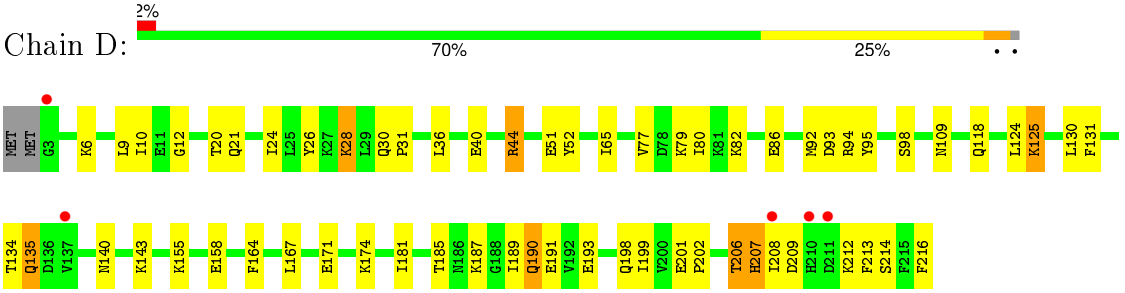
- Molecule 1: THYMIDYLATE KINASE

Chain C:



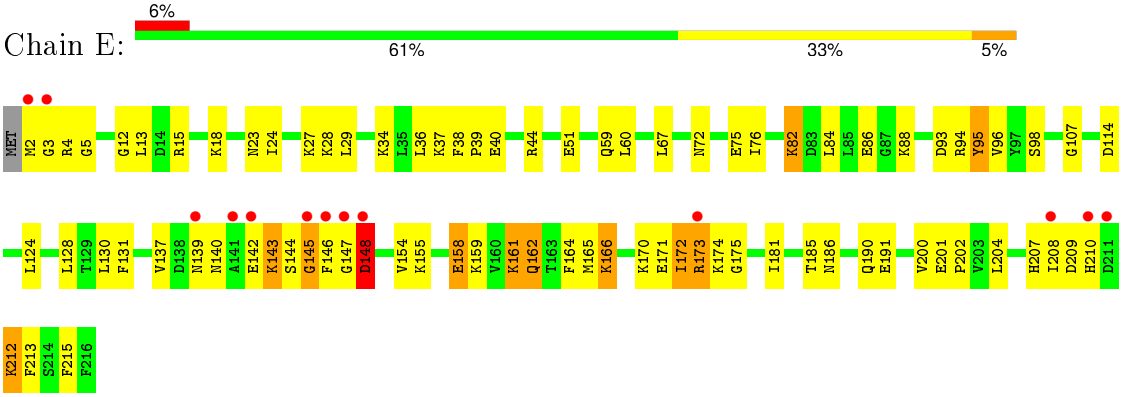
- Molecule 1: THYMIDYLATE KINASE

Chain D:



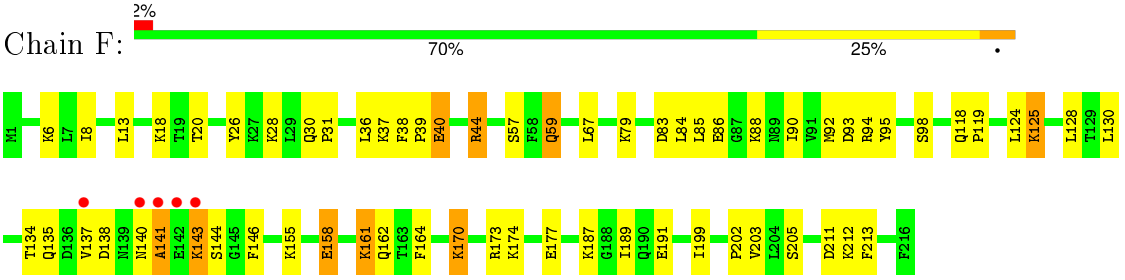
• Molecule 1: THYMIDYLATE KINASE

Chain E:



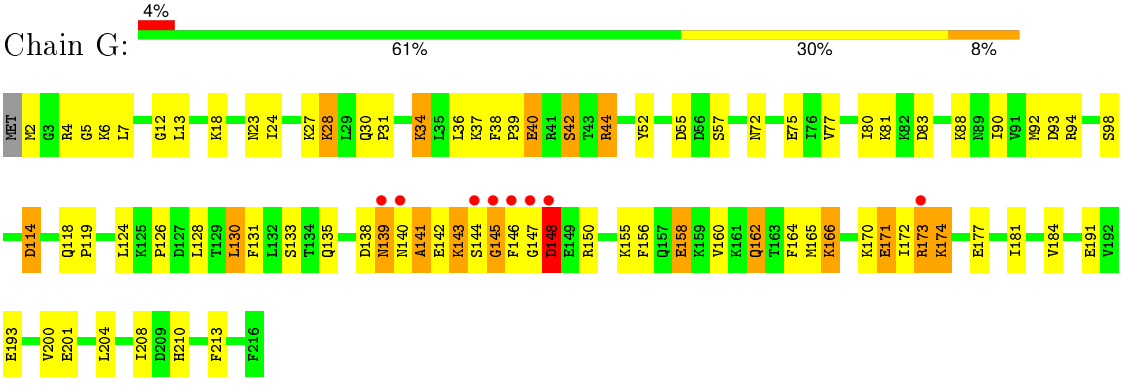
• Molecule 1: THYMIDYLATE KINASE

Chain F:



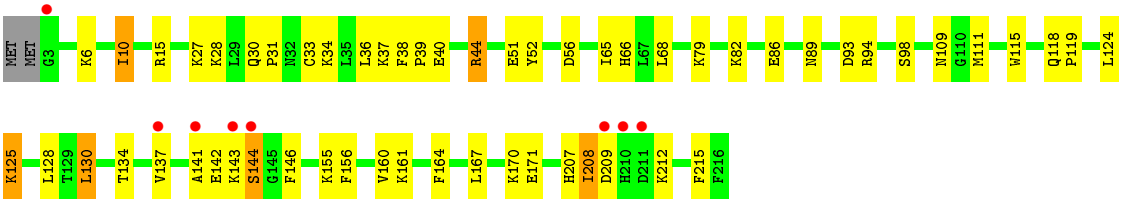
• Molecule 1: THYMIDYLATE KINASE

Chain G:



• Molecule 1: THYMIDYLATE KINASE

Chain H:


MET MET G3 K6 I10 R15 K27 K28 L29 Q30 P31 N32 C33 K34 L35 L36 K37 F38 P39 E40 R44 E51 Y52 D56 I65 H66 L67 L68 K79 K82 E86 N89 D93 R94 S98 N109 G110 M111 W115 Q118 P119 L124
K125 L128 T129 L130 T134 V137 A141 E142 K143 S144 G145 F146 K155 F156 V160 K161 F164 L167 K170 E171 H207 I208 D209 H210 D211 K212 F215 F216

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.57Å 87.32Å 155.02Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	43.80 – 2.00 43.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.80-2.00) 82.0 (43.66-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.279 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	1.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 64.6	EDS
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Outliers	7 of 107333 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15240	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.18 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1888e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: T5A

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	0.49	0/1765	0.68	0/2375
1	B	0.48	0/1762	0.67	0/2371
1	C	0.55	1/1684 (0.1%)	0.71	1/2265 (0.0%)
1	D	0.48	0/1736	0.65	0/2338
1	E	0.47	0/1750	0.65	0/2356
1	F	0.49	0/1758	0.67	0/2366
1	G	0.46	0/1750	0.67	0/2356
1	H	0.49	0/1735	0.67	0/2338
All	All	0.49	1/13940 (0.0%)	0.67	1/18765 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	ASP	C-N	9.34	1.55	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	148	ASP	C-N-CA	-5.75	107.32	121.70

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	1736	0	1757	98	1
1	B	1733	0	1755	42	0
1	C	1657	0	1687	113	0
1	D	1707	0	1724	53	0
1	E	1722	0	1738	79	0
1	F	1729	0	1749	44	1
1	G	1722	0	1738	78	0
1	H	1706	0	1715	43	0
2	A	55	0	25	1	0
2	B	55	0	25	1	0
2	C	55	0	25	3	0
2	D	55	0	25	0	0
2	E	55	0	25	1	0
2	F	55	0	25	0	0
2	G	55	0	25	0	0
2	H	55	0	25	1	0
3	A	129	0	0	12	0
3	B	161	0	0	13	0
3	C	134	0	0	10	0
3	D	144	0	0	13	0
3	E	126	0	0	14	0
3	F	147	0	0	14	0
3	G	136	0	0	17	0
3	H	111	0	0	8	0
All	All	15240	0	14063	535	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (535) 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:162:GLN:H	1:C:162:GLN:NE2	1.33	1.24
1:C:162:GLN:HE21	1:C:162:GLN:N	1.44	1.12
1:A:2:MET:HG3	1:A:3:GLY:H	1.08	1.11
1:D:44:ARG:HG2	3:D:4143:HOH:O	1.51	1.10
1:H:44:ARG:HG3	1:H:44:ARG:HH11	1.15	1.09
1:E:139:ASN:HA	3:E:4681:HOH:O	1.56	1.05
1:G:200:VAL:HG12	1:G:204:LEU:HD11	1.41	0.99
1:E:13:LEU:HD11	1:E:161:LYS:HG3	1.44	0.98
1:H:134:THR:HG22	3:H:4688:HOH:O	1.63	0.98
1:A:162:GLN:N	1:A:162:GLN:HE21	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LYS:HB2	1:C:174:LYS:NZ	1.80	0.97
1:B:37:LYS:HE3	3:B:4579:HOH:O	1.64	0.97
1:G:147:GLY:O	1:G:148:ASP:HB2	1.63	0.96
1:D:6:LYS:HD2	1:D:208:ILE:HD11	1.47	0.95
1:G:200:VAL:CG1	1:G:204:LEU:HD11	1.97	0.94
1:F:44:ARG:HG2	3:F:4965:HOH:O	1.65	0.94
1:C:190:GLN:HG2	3:C:5001:HOH:O	1.67	0.93
1:G:28:LYS:HE3	3:G:5321:HOH:O	1.69	0.92
1:C:174:LYS:HB2	1:C:174:LYS:HZ3	1.31	0.92
1:A:2:MET:HG3	1:A:3:GLY:N	1.83	0.91
1:E:162:GLN:H	1:E:162:GLN:HE21	0.97	0.91
1:E:15:ARG:HG2	1:E:143:LYS:HA	1.51	0.91
1:H:10:ILE:HD11	1:H:130:LEU:HD12	1.50	0.91
1:A:162:GLN:H	1:A:162:GLN:HE21	0.99	0.90
1:A:200:VAL:CG1	1:A:204:LEU:HD11	2.00	0.90
1:B:161:LYS:HD2	3:B:4437:HOH:O	1.72	0.89
1:C:200:VAL:HG12	1:C:204:LEU:CD2	2.03	0.88
1:A:146:PHE:H	1:A:146:PHE:HD1	1.21	0.88
1:E:158:GLU:O	1:E:162:GLN:NE2	2.06	0.88
1:A:200:VAL:HG12	1:A:204:LEU:CD1	2.02	0.88
1:E:147:GLY:O	1:E:148:ASP:HB2	1.72	0.88
1:H:10:ILE:CD1	1:H:130:LEU:HD12	2.04	0.87
1:C:153:THR:HB	1:C:156:PHE:HB3	1.53	0.87
1:C:13:LEU:HD11	1:C:161:LYS:HD2	1.55	0.87
1:A:200:VAL:HG12	1:A:204:LEU:HD11	1.54	0.86
1:G:200:VAL:HG12	1:G:204:LEU:CD1	2.05	0.86
1:G:166:LYS:HD3	1:G:170:LYS:HE3	1.57	0.86
1:A:146:PHE:N	1:A:146:PHE:CD1	2.41	0.85
1:C:155:LYS:O	1:C:159:LYS:HD3	1.78	0.84
1:C:159:LYS:H	1:C:159:LYS:HD2	1.41	0.83
1:H:44:ARG:HG3	1:H:44:ARG:NH1	1.86	0.83
1:G:200:VAL:O	1:G:204:LEU:HD12	1.79	0.82
1:D:28:LYS:HE3	3:D:4223:HOH:O	1.77	0.82
1:E:162:GLN:N	1:E:162:GLN:HE21	1.77	0.82
1:A:166:LYS:O	1:A:170:LYS:HG3	1.80	0.81
1:A:146:PHE:N	1:A:146:PHE:HD1	1.76	0.81
1:E:200:VAL:CG1	1:E:204:LEU:HD11	2.11	0.81
1:A:131:PHE:HB3	1:A:181:ILE:HD12	1.61	0.81
1:G:171:GLU:HG2	3:G:4576:HOH:O	1.78	0.81
1:A:2:MET:CG	1:A:3:GLY:H	1.92	0.80
1:H:6:LYS:HE3	1:H:208:ILE:HG13	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ASN:O	1:E:27:LYS:HD2	1.82	0.80
1:A:5:GLY:HA3	1:A:88:LYS:O	1.83	0.79
1:C:156:PHE:O	1:C:159:LYS:HG2	1.83	0.78
1:C:159:LYS:N	1:C:159:LYS:HD2	1.99	0.78
1:C:13:LEU:CD2	1:C:160:VAL:HG22	2.15	0.77
1:G:173:ARG:HG3	1:G:173:ARG:O	1.84	0.76
1:F:37:LYS:HG3	3:F:4841:HOH:O	1.85	0.76
1:G:171:GLU:HG3	3:G:5194:HOH:O	1.85	0.76
1:B:203:VAL:HG23	3:B:4786:HOH:O	1.85	0.75
1:D:6:LYS:CD	1:D:208:ILE:HD11	2.16	0.75
1:E:143:LYS:C	1:E:145:GLY:H	1.90	0.75
1:H:167:LEU:O	1:H:171:GLU:HG2	1.87	0.75
1:C:37:LYS:HG3	3:C:4946:HOH:O	1.86	0.74
1:A:137:VAL:HG23	3:A:4743:HOH:O	1.88	0.74
1:E:212:LYS:HD2	1:E:213:PHE:N	2.03	0.74
1:D:82:LYS:O	1:D:86:GLU:HG3	1.87	0.74
1:G:36:LEU:CD2	1:G:80:ILE:HD11	2.18	0.74
1:C:212:LYS:C	1:C:212:LYS:HD3	2.07	0.74
1:H:6:LYS:CD	1:H:208:ILE:HD11	2.18	0.74
1:E:172:ILE:HG12	3:E:4898:HOH:O	1.87	0.74
1:A:172:ILE:HG22	1:A:173:ARG:N	2.03	0.74
1:A:165:MET:HG2	3:A:4689:HOH:O	1.86	0.74
1:C:200:VAL:CG1	1:C:204:LEU:CD2	2.67	0.73
1:D:124:LEU:HD21	1:D:213:PHE:CD1	2.22	0.73
1:G:36:LEU:HD21	1:G:80:ILE:HD11	1.70	0.72
1:E:200:VAL:HG12	1:E:204:LEU:HD11	1.71	0.72
1:A:170:LYS:O	1:A:174:LYS:HB2	1.90	0.72
1:C:154:VAL:O	1:C:158:GLU:HG3	1.89	0.72
1:H:27:LYS:HE2	3:H:4805:HOH:O	1.89	0.72
1:C:31:PRO:HD2	3:C:4458:HOH:O	1.89	0.71
1:B:136:ASP:OD2	1:B:139:ASN:HB3	1.89	0.71
1:B:44:ARG:HG2	3:B:4605:HOH:O	1.89	0.71
1:C:162:GLN:NE2	1:C:162:GLN:N	2.18	0.71
1:E:200:VAL:HG12	1:E:204:LEU:CD1	2.21	0.70
1:C:187:LYS:HG3	1:C:191:GLU:CD	2.12	0.70
1:B:208:ILE:HG22	1:B:209:ASP:CG	2.12	0.70
1:H:141:ALA:HA	1:H:146:PHE:CD2	2.27	0.70
1:C:156:PHE:HA	1:C:159:LYS:HD3	1.74	0.70
1:D:209:ASP:HB2	1:D:212:LYS:CB	2.22	0.69
1:B:162:GLN:HG3	3:B:5155:HOH:O	1.92	0.69
1:A:173:ARG:O	1:A:173:ARG:HG3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:H	1:A:162:GLN:NE2	1.83	0.69
1:C:13:LEU:HD21	1:C:160:VAL:HG22	1.72	0.69
1:F:125:LYS:HE3	3:F:4275:HOH:O	1.92	0.69
1:A:13:LEU:HD11	1:A:161:LYS:HG3	1.74	0.69
1:G:166:LYS:O	1:G:170:LYS:HG3	1.93	0.68
1:C:13:LEU:CD1	1:C:161:LYS:HD2	2.23	0.68
1:A:167:LEU:HD12	1:A:167:LEU:O	1.94	0.68
1:E:166:LYS:O	1:E:170:LYS:HG3	1.93	0.68
1:C:153:THR:HB	1:C:156:PHE:CB	2.22	0.68
1:C:210:HIS:HE1	3:C:4490:HOH:O	1.76	0.67
1:G:210:HIS:HE1	3:G:4867:HOH:O	1.77	0.67
1:A:44:ARG:HH22	1:B:51:GLU:CD	1.99	0.67
1:G:131:PHE:HB3	1:G:181:ILE:HD12	1.76	0.66
1:F:83:ASP:OD2	3:F:4280:HOH:O	2.13	0.66
1:D:174:LYS:O	3:D:5295:HOH:O	2.13	0.66
1:H:93:ASP:O	1:H:94:ARG:HB2	1.94	0.66
1:A:2:MET:HG3	1:A:210:HIS:HB2	1.77	0.66
1:D:190:GLN:HG2	3:G:5294:HOH:O	1.96	0.66
1:H:6:LYS:HD2	1:H:208:ILE:HD11	1.78	0.66
1:F:86:GLU:OE1	1:F:88:LYS:HE3	1.96	0.66
1:E:172:ILE:HG22	1:E:173:ARG:N	2.11	0.65
1:G:143:LYS:HG3	1:G:145:GLY:H	1.61	0.65
1:D:51:GLU:OE1	3:D:4213:HOH:O	2.15	0.65
1:C:159:LYS:N	1:C:159:LYS:CD	2.60	0.65
1:G:200:VAL:O	1:G:204:LEU:CD1	2.45	0.65
1:H:6:LYS:HE3	1:H:208:ILE:CG1	2.26	0.65
1:G:12:GLY:HA2	1:G:131:PHE:CE1	2.32	0.65
1:E:207:HIS:O	3:E:4951:HOH:O	2.14	0.64
1:H:34:LYS:NZ	3:H:5030:HOH:O	2.29	0.64
1:C:212:LYS:HD3	1:C:213:PHE:N	2.13	0.64
1:C:162:GLN:H	1:C:162:GLN:HE21	0.70	0.64
1:B:191:GLU:OE2	1:E:191:GLU:CG	2.45	0.64
1:D:209:ASP:HB2	1:D:212:LYS:HB3	1.81	0.63
1:D:6:LYS:CD	1:D:208:ILE:CD1	2.77	0.63
1:E:173:ARG:HG3	1:E:173:ARG:O	1.97	0.63
1:E:82:LYS:O	1:E:86:GLU:HG3	1.97	0.63
1:A:158:GLU:O	1:A:162:GLN:NE2	2.31	0.63
1:E:200:VAL:O	1:E:204:LEU:CD1	2.46	0.63
1:G:23:ASN:O	1:G:27:LYS:HD2	1.98	0.63
1:D:9:LEU:C	1:D:10:ILE:HD12	2.20	0.63
1:G:171:GLU:CG	3:G:5194:HOH:O	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:NE2	3:A:4830:HOH:O	2.32	0.62
1:C:167:LEU:HD12	1:C:170:LYS:HD3	1.81	0.62
1:A:15:ARG:HB3	1:A:142:GLU:HB3	1.80	0.62
1:A:30:GLN:HG2	1:A:31:PRO:HA	1.82	0.62
1:E:147:GLY:O	1:E:148:ASP:CB	2.46	0.61
1:A:140:ASN:OD1	1:A:143:LYS:HE3	2.01	0.61
1:C:124:LEU:HD22	1:C:213:PHE:CD1	2.36	0.61
1:D:216:PHE:HD1	3:D:4879:HOH:O	1.81	0.61
1:G:172:ILE:HG22	1:G:173:ARG:N	2.15	0.61
1:C:12:GLY:HA2	1:C:131:PHE:CE1	2.35	0.61
1:B:72:ASN:O	1:B:76:ILE:HD12	2.01	0.61
1:A:146:PHE:O	1:A:148:ASP:N	2.29	0.61
1:C:131:PHE:HB3	1:C:181:ILE:HD12	1.83	0.61
1:D:191:GLU:OE2	1:G:191:GLU:OE2	2.17	0.61
1:D:134:THR:HG21	1:D:140:ASN:HD21	1.66	0.61
1:B:139:ASN:O	1:B:142:GLU:HB2	2.00	0.60
1:C:34:LYS:HA	3:C:5086:HOH:O	2.01	0.60
1:A:130:LEU:HD11	1:A:199:ILE:HG21	1.82	0.60
1:C:125:LYS:NZ	1:C:171:GLU:OE2	2.27	0.60
1:G:2:MET:N	3:G:5235:HOH:O	2.35	0.60
1:G:34:LYS:HD2	1:G:88:LYS:HD2	1.83	0.60
1:E:131:PHE:HB3	1:E:181:ILE:HD12	1.84	0.60
1:B:93:ASP:O	1:B:94:ARG:HB2	2.03	0.59
1:G:13:LEU:O	1:G:18:LYS:NZ	2.34	0.59
1:C:169:ASP:HB3	1:C:173:ARG:NH2	2.17	0.59
1:F:143:LYS:HG2	3:F:5096:HOH:O	2.02	0.59
1:A:200:VAL:O	1:A:204:LEU:CD1	2.50	0.59
1:B:3:GLY:HA3	1:B:207:HIS:CE1	2.37	0.59
1:C:30:GLN:HG2	1:C:31:PRO:HA	1.83	0.59
1:B:208:ILE:HG22	1:B:209:ASP:OD2	2.02	0.59
1:B:191:GLU:OE2	1:E:191:GLU:OE2	2.19	0.59
1:C:158:GLU:O	1:C:162:GLN:NE2	2.33	0.59
1:C:200:VAL:HG12	1:C:204:LEU:HD22	1.84	0.59
1:A:28:LYS:HD2	3:A:4971:HOH:O	2.01	0.59
1:E:166:LYS:CE	1:E:170:LYS:HE3	2.32	0.59
1:B:167:LEU:O	1:B:171:GLU:HG2	2.03	0.59
1:A:93:ASP:O	1:A:94:ARG:HB2	2.02	0.58
1:C:37:LYS:CG	3:C:4946:HOH:O	2.45	0.58
1:D:10:ILE:N	1:D:10:ILE:HD12	2.19	0.58
1:H:10:ILE:HD12	1:H:130:LEU:HD12	1.86	0.58
1:E:142:GLU:O	2:E:217:T5A:HA51	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:HD3	1:A:139:ASN:O	2.04	0.58
1:C:181:ILE:N	1:C:181:ILE:HD13	2.19	0.58
1:E:72:ASN:O	1:E:76:ILE:HD12	2.03	0.58
1:B:37:LYS:HG3	1:B:93:ASP:HB3	1.86	0.58
1:E:13:LEU:CD1	1:E:161:LYS:HG3	2.27	0.57
1:B:141:ALA:HA	1:B:146:PHE:CD2	2.39	0.57
1:A:36:LEU:HD12	1:A:37:LYS:H	1.69	0.57
1:C:29:LEU:HB3	3:C:4202:HOH:O	2.05	0.57
1:C:161:LYS:HB3	1:C:162:GLN:HE21	1.70	0.57
1:C:13:LEU:O	1:C:18:LYS:NZ	2.36	0.57
1:A:200:VAL:HG12	1:A:204:LEU:HD13	1.85	0.57
1:C:36:LEU:CD2	1:C:80:ILE:HD11	2.33	0.57
1:F:130:LEU:HD21	1:F:199:ILE:HG21	1.86	0.57
1:C:161:LYS:HB3	1:C:162:GLN:NE2	2.20	0.57
1:C:18:LYS:HE2	3:C:4181:HOH:O	2.05	0.57
1:D:21:GLN:OE1	3:D:4168:HOH:O	2.17	0.57
1:A:200:VAL:CG1	1:A:204:LEU:CD1	2.71	0.57
1:G:55:ASP:OD1	1:G:57:SER:HB2	2.04	0.57
1:E:67:LEU:HD22	1:F:67:LEU:HD22	1.87	0.57
1:C:23:ASN:O	1:C:27:LYS:HD2	2.05	0.57
1:C:155:LYS:HA	1:C:158:GLU:OE2	2.04	0.57
1:C:158:GLU:OE1	1:C:159:LYS:NZ	2.38	0.56
1:E:143:LYS:O	1:E:143:LYS:HG2	2.06	0.56
1:C:174:LYS:HB2	1:C:174:LYS:HZ2	1.69	0.56
1:A:180:THR:HG21	1:A:199:ILE:HD13	1.87	0.56
1:C:155:LYS:HA	1:C:158:GLU:CD	2.25	0.56
1:B:206:THR:HG22	1:B:207:HIS:N	2.20	0.56
1:E:181:ILE:HD13	1:E:181:ILE:N	2.21	0.56
1:C:151:TYR:O	1:C:153:THR:N	2.37	0.56
1:E:166:LYS:HE2	1:E:170:LYS:HE3	1.88	0.56
1:E:143:LYS:C	1:E:145:GLY:N	2.59	0.56
1:C:149:GLU:H	1:C:152:GLU:HG3	1.70	0.56
1:C:136:ASP:OD1	1:C:136:ASP:N	2.38	0.56
1:G:141:ALA:O	1:G:143:LYS:N	2.39	0.55
1:C:200:VAL:CG1	1:C:204:LEU:HD22	2.37	0.55
1:C:173:ARG:HD3	1:C:173:ARG:N	2.21	0.55
1:H:109:ASN:ND2	3:H:4704:HOH:O	2.38	0.55
1:A:183:ASP:O	1:A:187:LYS:HE2	2.06	0.55
1:C:155:LYS:O	1:C:159:LYS:CD	2.52	0.55
1:B:206:THR:HG22	1:B:207:HIS:H	1.71	0.55
1:H:209:ASP:HB2	1:H:212:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:HD2	3:A:4691:HOH:O	2.06	0.55
1:G:171:GLU:CG	3:G:4576:HOH:O	2.48	0.55
1:E:124:LEU:HD21	1:E:213:PHE:CD1	2.42	0.55
1:F:155:LYS:HD3	3:F:5173:HOH:O	2.06	0.55
1:F:128:LEU:HD22	1:F:203:VAL:HG21	1.89	0.55
1:G:162:GLN:N	1:G:162:GLN:HE21	2.04	0.55
1:E:137:VAL:HG11	1:E:158:GLU:OE1	2.08	0.54
1:D:6:LYS:HD2	1:D:208:ILE:CD1	2.27	0.54
1:D:209:ASP:HB2	1:D:212:LYS:HB2	1.88	0.54
1:D:93:ASP:O	1:D:94:ARG:HB2	2.08	0.54
1:F:93:ASP:O	1:F:94:ARG:HB2	2.07	0.54
1:G:52:TYR:O	1:G:150:ARG:NH1	2.37	0.54
1:C:40:GLU:OE1	1:C:42:SER:HB3	2.07	0.54
1:D:6:LYS:HE3	1:D:208:ILE:HG13	1.89	0.54
1:G:7:LEU:HD23	1:G:126:PRO:HA	1.90	0.54
1:E:175:GLY:C	3:E:4949:HOH:O	2.45	0.54
1:A:148:ASP:OD1	1:A:152:GLU:HB2	2.08	0.54
1:E:200:VAL:HG13	1:E:204:LEU:HD11	1.88	0.54
1:D:207:HIS:HA	3:D:4677:HOH:O	2.08	0.54
1:A:140:ASN:O	1:A:143:LYS:HD2	2.09	0.53
1:D:198:GLN:HG3	3:D:4417:HOH:O	2.08	0.53
1:G:83:ASP:HB2	1:G:90:ILE:HD11	1.90	0.53
1:C:171:GLU:O	1:C:176:ASP:HB3	2.08	0.53
1:A:52:TYR:CE2	1:A:150:ARG:HD3	2.44	0.53
1:B:111:MET:HG2	1:B:115:TRP:CZ3	2.43	0.53
1:C:156:PHE:O	1:C:159:LYS:CG	2.57	0.52
1:H:44:ARG:CG	1:H:44:ARG:HH11	1.99	0.52
1:C:200:VAL:CG1	1:C:204:LEU:HD21	2.39	0.52
1:A:131:PHE:HB3	1:A:181:ILE:CD1	2.35	0.52
1:C:81:LYS:CG	1:C:124:LEU:HD11	2.39	0.52
1:A:162:GLN:N	1:A:162:GLN:NE2	2.43	0.52
1:G:114:ASP:HB2	3:G:4522:HOH:O	2.10	0.52
1:A:199:ILE:O	1:A:202:PRO:HD2	2.10	0.52
1:E:170:LYS:O	1:E:174:LYS:HB2	2.09	0.52
1:D:125:LYS:HD3	3:D:4889:HOH:O	2.09	0.52
1:B:37:LYS:HG2	3:B:4579:HOH:O	2.08	0.52
1:A:113:LEU:HD11	1:A:166:LYS:HD2	1.91	0.52
1:C:187:LYS:HB3	1:C:192:VAL:HG23	1.92	0.52
1:C:5:GLY:HA3	1:C:88:LYS:O	2.09	0.52
1:E:3:GLY:HA2	1:E:208:ILE:O	2.09	0.52
1:G:93:ASP:O	1:G:94:ARG:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:THR:OG1	2:C:217:T5A:HA8	2.09	0.52
1:C:7:LEU:HD23	1:C:126:PRO:HA	1.92	0.52
1:F:189:ILE:HD12	3:F:5031:HOH:O	2.10	0.52
1:C:168:LEU:HD22	1:C:179:ILE:HG21	1.92	0.51
1:G:6:LYS:HE2	3:G:5264:HOH:O	2.11	0.51
1:C:52:TYR:O	1:C:150:ARG:HD2	2.10	0.51
1:H:125:LYS:HD3	3:H:4364:HOH:O	2.09	0.51
1:G:37:LYS:HG3	3:G:4928:HOH:O	2.10	0.51
1:F:57:SER:O	1:F:59:GLN:HG2	2.10	0.51
1:G:143:LYS:HD3	3:G:5247:HOH:O	2.11	0.51
1:E:5:GLY:HA3	1:E:88:LYS:O	2.11	0.50
1:C:171:GLU:HA	1:C:171:GLU:OE1	2.10	0.50
1:G:143:LYS:HG3	1:G:145:GLY:N	2.26	0.50
1:D:118:GLN:HB2	3:D:4718:HOH:O	2.11	0.50
1:F:8:ILE:N	1:F:8:ILE:HD12	2.26	0.50
1:D:24:ILE:HG21	1:D:193:GLU:HG3	1.93	0.50
1:C:169:ASP:HB3	1:C:173:ARG:CZ	2.41	0.50
1:E:12:GLY:HA2	1:E:131:PHE:CE1	2.47	0.50
1:B:13:LEU:O	1:B:18:LYS:NZ	2.41	0.50
1:A:67:LEU:HD22	1:B:67:LEU:HD22	1.94	0.50
1:B:44:ARG:NE	3:B:4566:HOH:O	2.42	0.50
1:C:156:PHE:HA	1:C:159:LYS:CD	2.40	0.50
1:E:166:LYS:HE3	1:E:170:LYS:HE3	1.94	0.50
1:A:7:LEU:HD23	1:A:126:PRO:HA	1.93	0.50
3:E:4777:HOH:O	1:F:118:GLN:HB2	2.11	0.49
1:A:4:ARG:HG2	1:A:210:HIS:HA	1.93	0.49
1:B:37:LYS:CG	3:B:4579:HOH:O	2.60	0.49
1:E:212:LYS:C	1:E:212:LYS:HD2	2.31	0.49
1:G:38:PHE:HA	1:G:39:PRO:C	2.32	0.49
1:B:84:LEU:HG	1:B:90:ILE:HD12	1.93	0.49
1:C:174:LYS:NZ	1:C:174:LYS:CB	2.56	0.49
1:E:200:VAL:O	1:E:204:LEU:HD13	2.11	0.49
1:H:109:ASN:HB2	3:H:4356:HOH:O	2.12	0.49
1:D:77:VAL:HA	1:D:80:ILE:HD12	1.94	0.49
1:B:191:GLU:OE2	1:E:191:GLU:HG2	2.12	0.49
1:C:167:LEU:CD1	1:C:170:LYS:HD3	2.43	0.49
1:A:36:LEU:HD12	1:A:37:LYS:N	2.26	0.49
1:E:143:LYS:O	1:E:145:GLY:N	2.45	0.48
1:F:203:VAL:HG23	3:F:4314:HOH:O	2.13	0.48
1:A:135:GLN:HG3	1:A:185:THR:HG21	1.94	0.48
1:G:166:LYS:HD3	1:G:170:LYS:CE	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:LYS:CD	1:H:208:ILE:CD1	2.91	0.48
1:E:107:GLY:HA3	1:G:2:MET:HB2	1.95	0.48
1:B:143:LYS:HE2	3:B:4784:HOH:O	2.13	0.48
1:A:137:VAL:CG2	3:A:4743:HOH:O	2.55	0.48
1:G:138:ASP:O	1:G:139:ASN:C	2.51	0.48
1:G:18:LYS:HB2	1:G:18:LYS:HE2	1.62	0.48
1:F:141:ALA:HA	1:F:146:PHE:CD1	2.47	0.48
1:E:200:VAL:O	1:E:204:LEU:HD12	2.12	0.48
1:G:181:ILE:HD13	1:G:181:ILE:N	2.28	0.48
1:A:200:VAL:O	1:A:204:LEU:HD12	2.13	0.48
1:F:37:LYS:CG	3:F:4841:HOH:O	2.51	0.48
1:E:37:LYS:HG3	3:E:4307:HOH:O	2.12	0.48
1:G:5:GLY:HA3	1:G:88:LYS:O	2.14	0.48
1:G:143:LYS:HB3	1:G:143:LYS:HE3	1.43	0.48
1:G:37:LYS:CG	3:G:4928:HOH:O	2.62	0.48
1:C:13:LEU:HD23	1:C:160:VAL:HG22	1.93	0.48
1:C:153:THR:CB	1:C:156:PHE:HB3	2.36	0.48
1:H:30:GLN:HB3	1:H:31:PRO:HA	1.95	0.48
1:H:156:PHE:O	1:H:160:VAL:HG23	2.14	0.47
1:A:144:SER:O	1:A:144:SER:OG	2.31	0.47
1:C:154:VAL:O	1:C:158:GLU:CG	2.61	0.47
1:E:38:PHE:HA	1:E:39:PRO:C	2.33	0.47
1:B:156:PHE:O	1:B:160:VAL:HG23	2.14	0.47
1:A:13:LEU:O	1:A:18:LYS:NZ	2.45	0.47
1:C:125:LYS:HZ3	1:C:171:GLU:HG3	1.79	0.47
1:B:15:ARG:O	1:B:140:ASN:ND2	2.47	0.47
1:C:79:LYS:HG2	3:C:5151:HOH:O	2.14	0.47
1:D:6:LYS:HE2	1:D:206:THR:O	2.14	0.47
1:E:143:LYS:HG3	1:E:145:GLY:CA	2.45	0.47
1:B:130:LEU:CD2	1:B:199:ILE:HG21	2.44	0.47
1:E:159:LYS:HD2	3:E:5377:HOH:O	2.15	0.47
1:E:28:LYS:NZ	3:E:4300:HOH:O	2.48	0.47
1:C:159:LYS:H	1:C:159:LYS:CD	2.09	0.47
1:C:148:ASP:OD1	1:C:152:GLU:CB	2.62	0.47
1:G:158:GLU:O	1:G:162:GLN:NE2	2.47	0.47
1:F:170:LYS:CD	3:F:4575:HOH:O	2.62	0.47
1:D:135:GLN:HB2	1:D:185:THR:HG21	1.96	0.47
1:H:38:PHE:HA	1:H:39:PRO:C	2.35	0.47
1:D:167:LEU:O	1:D:171:GLU:HG2	2.15	0.47
1:A:172:ILE:C	1:A:174:LYS:H	2.18	0.47
1:E:37:LYS:CG	3:E:4307:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MET:CG	1:A:210:HIS:HB2	2.45	0.47
1:A:200:VAL:O	1:A:204:LEU:HD13	2.13	0.47
1:C:134:THR:O	1:C:161:LYS:NZ	2.37	0.47
1:D:44:ARG:HH11	1:D:44:ARG:HB3	1.80	0.47
1:C:36:LEU:O	1:C:92:MET:HA	2.15	0.47
1:C:4:ARG:CZ	1:C:208:ILE:HG21	2.45	0.47
1:A:136:ASP:O	1:A:137:VAL:O	2.33	0.46
1:A:18:LYS:HB2	1:A:18:LYS:HE2	1.68	0.46
1:A:133:SER:O	1:A:184:VAL:HG22	2.16	0.46
1:E:93:ASP:O	1:E:94:ARG:HB2	2.15	0.46
1:A:37:LYS:HG3	3:A:4084:HOH:O	2.15	0.46
1:E:201:GLU:N	1:E:202:PRO:HD2	2.31	0.46
1:F:40:GLU:C	1:F:40:GLU:OE1	2.53	0.46
1:D:30:GLN:HB3	1:D:31:PRO:HA	1.97	0.46
1:A:15:ARG:HD2	1:A:138:ASP:O	2.15	0.46
1:G:144:SER:O	1:G:145:GLY:O	2.33	0.46
1:D:191:GLU:OE2	1:G:191:GLU:CG	2.64	0.46
1:G:162:GLN:H	1:G:162:GLN:HE21	1.62	0.46
1:B:190:GLN:HG2	3:E:4599:HOH:O	2.16	0.46
1:F:13:LEU:HD11	1:F:161:LYS:HB2	1.97	0.46
1:F:20:THR:HG21	1:F:189:ILE:HG12	1.97	0.46
3:B:4336:HOH:O	1:E:28:LYS:HD3	2.15	0.46
1:A:44:ARG:CG	3:A:4603:HOH:O	2.64	0.46
1:A:55:ASP:OD1	1:A:57:SER:HB2	2.16	0.46
1:E:36:LEU:HD12	1:E:37:LYS:N	2.30	0.46
1:G:44:ARG:NH1	3:G:5129:HOH:O	2.48	0.46
1:C:38:PHE:HA	1:C:39:PRO:C	2.36	0.46
1:G:72:ASN:O	1:G:75:GLU:HG2	2.15	0.46
1:E:29:LEU:HB3	3:E:4316:HOH:O	2.15	0.46
1:F:30:GLN:HB3	1:F:31:PRO:HA	1.98	0.46
1:A:2:MET:O	1:A:207:HIS:HE1	1.99	0.46
1:D:201:GLU:OE2	1:G:201:GLU:OE2	2.33	0.46
1:C:148:ASP:OD1	1:C:152:GLU:HB3	2.15	0.46
1:H:52:TYR:CD2	1:H:65:ILE:HG12	2.51	0.46
1:C:189:ILE:HG12	2:C:217:T5A:N7A	2.31	0.45
1:H:52:TYR:CE2	1:H:65:ILE:HG12	2.51	0.45
1:H:36:LEU:HD12	1:H:37:LYS:H	1.81	0.45
1:D:10:ILE:N	1:D:10:ILE:CD1	2.79	0.45
1:F:143:LYS:HG3	1:F:144:SER:H	1.81	0.45
1:F:170:LYS:HE2	3:F:4575:HOH:O	2.15	0.45
1:H:65:ILE:HG23	1:H:66:HIS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG21	1:A:199:ILE:CD1	2.46	0.45
1:D:20:THR:HG21	1:D:189:ILE:HG12	1.97	0.45
1:D:189:ILE:HD12	3:D:4597:HOH:O	2.16	0.45
1:G:124:LEU:CD2	1:G:213:PHE:HB3	2.47	0.45
1:E:4:ARG:HB2	1:E:84:LEU:O	2.16	0.45
1:C:36:LEU:HD21	1:C:80:ILE:HD11	1.97	0.45
1:A:146:PHE:HD2	3:A:4692:HOH:O	1.99	0.45
1:C:84:LEU:HG	1:C:90:ILE:HD12	1.99	0.45
1:G:156:PHE:O	1:G:160:VAL:HG23	2.16	0.45
1:A:4:ARG:CZ	1:A:208:ILE:HG21	2.47	0.45
1:G:118:GLN:HB2	1:G:119:PRO:HD3	1.99	0.45
1:A:2:MET:HG2	1:A:210:HIS:HB3	1.99	0.45
1:G:18:LYS:HE2	3:G:4413:HOH:O	2.17	0.45
1:C:8:ILE:HD12	1:C:128:LEU:HD23	1.98	0.45
1:D:201:GLU:HB3	1:D:202:PRO:HD3	1.97	0.45
1:E:44:ARG:HG2	1:E:44:ARG:H	1.62	0.45
1:E:209:ASP:HB3	1:E:212:LYS:HB2	1.98	0.45
1:A:14:ASP:OD2	1:A:157:GLN:NE2	2.45	0.45
1:H:137:VAL:O	1:H:137:VAL:HG12	2.17	0.45
1:A:85:LEU:HD22	1:A:210:HIS:CE1	2.52	0.44
1:H:44:ARG:NH1	1:H:44:ARG:CG	2.62	0.44
1:C:1:MET:HB2	1:C:1:MET:HE2	1.79	0.44
1:H:134:THR:CG2	3:H:4688:HOH:O	2.41	0.44
1:H:15:ARG:NE	3:H:4430:HOH:O	2.44	0.44
1:E:200:VAL:CG1	1:E:204:LEU:CD1	2.83	0.44
1:E:95:TYR:CG	1:E:96:VAL:N	2.86	0.44
1:A:146:PHE:C	1:A:148:ASP:H	2.16	0.44
1:G:128:LEU:HD21	1:G:130:LEU:HD21	2.00	0.44
1:E:51:GLU:OE2	1:F:44:ARG:NH2	2.50	0.44
1:A:201:GLU:N	1:A:202:PRO:CD	2.81	0.44
1:G:24:ILE:HG21	1:G:193:GLU:HG3	1.99	0.44
1:G:77:VAL:O	1:G:77:VAL:HG22	2.18	0.44
1:D:44:ARG:HG2	1:D:44:ARG:H	1.56	0.44
1:C:37:LYS:NZ	2:C:217:T5A:O2X	2.51	0.44
1:C:86:GLU:OE1	1:C:88:LYS:HE3	2.18	0.44
1:E:24:ILE:HG23	3:E:4318:HOH:O	2.18	0.44
1:C:173:ARG:HD3	1:C:173:ARG:H	1.82	0.43
1:B:184:VAL:HB	3:B:4646:HOH:O	2.18	0.43
1:H:128:LEU:HD21	1:H:130:LEU:HD21	1.99	0.43
1:A:200:VAL:HG13	1:A:204:LEU:HD11	1.90	0.43
1:C:149:GLU:N	1:C:152:GLU:HG3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:GLN:HB2	1:F:119:PRO:HD3	1.99	0.43
1:F:26:TYR:O	1:F:30:GLN:HG3	2.18	0.43
1:H:118:GLN:HB2	1:H:119:PRO:HD3	1.99	0.43
1:B:47:GLY:O	1:B:51:GLU:HG3	2.19	0.43
1:B:143:LYS:HE3	2:B:217:T5A:O4F	2.18	0.43
1:G:40:GLU:OE1	1:G:42:SER:HB3	2.18	0.43
1:G:143:LYS:C	1:G:145:GLY:H	2.21	0.43
1:C:172:ILE:HG22	1:C:173:ARG:N	2.32	0.43
1:A:142:GLU:O	2:A:217:T5A:HA51	2.19	0.43
1:E:72:ASN:O	1:E:75:GLU:HG2	2.18	0.43
1:G:30:GLN:HG2	1:G:31:PRO:HA	2.01	0.43
1:F:134:THR:HG21	1:F:140:ASN:HD21	1.83	0.43
1:G:201:GLU:HA	1:G:204:LEU:HD13	2.01	0.43
1:H:6:LYS:HD3	1:H:208:ILE:CD1	2.49	0.43
1:A:44:ARG:NH2	1:B:51:GLU:CD	2.68	0.43
1:C:44:ARG:NH2	1:D:51:GLU:OE2	2.46	0.43
1:F:199:ILE:O	1:F:202:PRO:HD2	2.19	0.43
1:F:13:LEU:O	1:F:18:LYS:NZ	2.48	0.43
1:A:209:ASP:O	1:A:212:LYS:N	2.45	0.43
1:A:86:GLU:HG3	3:A:4452:HOH:O	2.19	0.43
1:H:82:LYS:O	1:H:86:GLU:HG3	2.19	0.43
1:A:138:ASP:HB2	1:A:154:VAL:CG2	2.49	0.43
1:A:38:PHE:HA	1:A:39:PRO:C	2.38	0.43
1:G:200:VAL:HG13	1:G:204:LEU:HD11	1.94	0.43
1:A:44:ARG:HG2	3:A:4603:HOH:O	2.19	0.43
1:C:1:MET:HB2	1:C:2:MET:H	1.71	0.43
1:C:174:LYS:CB	1:C:174:LYS:HZ3	2.15	0.42
1:A:172:ILE:C	1:A:174:LYS:N	2.72	0.42
1:C:34:LYS:HD2	1:C:88:LYS:HD2	2.01	0.42
1:D:36:LEU:O	1:D:92:MET:HA	2.19	0.42
3:B:4313:HOH:O	1:E:190:GLN:CG	2.67	0.42
1:A:15:ARG:CB	1:A:142:GLU:HB3	2.48	0.42
1:A:154:VAL:O	1:A:158:GLU:HB2	2.18	0.42
1:A:131:PHE:CB	1:A:181:ILE:HD12	2.41	0.42
1:G:81:LYS:HG3	1:G:124:LEU:HD11	2.00	0.42
1:F:36:LEU:HD21	1:F:38:PHE:CE2	2.54	0.42
1:C:95:TYR:CG	1:C:96:VAL:N	2.86	0.42
1:G:172:ILE:C	1:G:174:LYS:H	2.21	0.42
1:C:127:ASP:O	1:C:178:SER:HB2	2.19	0.42
1:F:158:GLU:HA	1:F:158:GLU:OE1	2.17	0.42
1:A:135:GLN:HG3	1:A:185:THR:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:CG	3:C:5151:HOH:O	2.66	0.42
1:F:174:LYS:O	3:F:4959:HOH:O	2.22	0.42
1:G:143:LYS:CD	3:G:5247:HOH:O	2.67	0.42
1:C:172:ILE:HG21	1:C:173:ARG:HH11	1.84	0.42
1:C:93:ASP:O	1:C:94:ARG:HB2	2.19	0.42
1:G:4:ARG:CZ	1:G:208:ILE:HG21	2.49	0.42
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.35	0.42
1:E:143:LYS:CG	1:E:145:GLY:H	2.33	0.42
1:D:124:LEU:CD2	1:D:213:PHE:CD1	3.01	0.42
1:G:139:ASN:O	1:G:141:ALA:O	2.38	0.42
1:A:124:LEU:HD23	1:A:215:PHE:CE1	2.54	0.42
1:F:85:LEU:HA	1:F:85:LEU:HD23	1.85	0.42
1:A:1:MET:SD	1:A:2:MET:HB2	2.60	0.42
1:A:166:LYS:HD3	1:A:170:LYS:HE3	2.01	0.42
1:G:52:TYR:CE1	1:G:150:ARG:HD3	2.55	0.42
1:E:128:LEU:CD1	3:E:4460:HOH:O	2.66	0.42
1:H:68:LEU:HA	1:H:68:LEU:HD23	1.85	0.42
1:C:171:GLU:CA	1:C:171:GLU:OE1	2.67	0.42
1:F:141:ALA:HA	1:F:146:PHE:CE1	2.55	0.42
1:C:130:LEU:HD11	1:C:199:ILE:HD13	2.02	0.42
1:E:18:LYS:HB2	1:E:18:LYS:HE2	1.77	0.42
1:C:51:GLU:OE2	1:D:44:ARG:NH2	2.53	0.41
1:F:158:GLU:OE2	1:F:162:GLN:NE2	2.53	0.41
1:F:84:LEU:HG	1:F:90:ILE:HD12	2.02	0.41
1:B:140:ASN:HD22	1:B:140:ASN:HA	1.59	0.41
1:F:38:PHE:HA	1:F:39:PRO:C	2.40	0.41
1:A:84:LEU:CD2	1:A:90:ILE:HD12	2.50	0.41
1:D:52:TYR:CD1	1:D:65:ILE:HG12	2.54	0.41
1:D:187:LYS:HD3	1:D:191:GLU:CD	2.41	0.41
1:F:36:LEU:O	1:F:92:MET:HA	2.20	0.41
1:B:149:GLU:HB2	1:B:152:GLU:CD	2.40	0.41
1:E:86:GLU:OE1	1:E:88:LYS:HE3	2.20	0.41
1:G:4:ARG:NH2	1:G:208:ILE:HG21	2.35	0.41
1:D:155:LYS:HD3	3:D:4441:HOH:O	2.20	0.41
1:E:200:VAL:HG12	1:E:204:LEU:HD13	2.00	0.41
1:E:44:ARG:HG2	3:E:4910:HOH:O	2.21	0.41
1:C:130:LEU:HD12	1:C:182:VAL:HG23	2.02	0.41
1:A:165:MET:HA	1:A:165:MET:CE	2.51	0.41
1:D:130:LEU:HD21	1:D:199:ILE:HG21	2.01	0.41
1:G:155:LYS:HG2	3:G:5210:HOH:O	2.19	0.41
1:F:177:GLU:HG2	3:F:5075:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MET:CG	1:A:210:HIS:CB	2.98	0.41
1:E:139:ASN:HB3	1:E:142:GLU:HB2	2.02	0.41
1:F:124:LEU:CD2	1:F:213:PHE:CD1	3.04	0.41
1:B:161:LYS:HZ3	1:B:165:MET:CE	2.33	0.41
1:G:36:LEU:O	1:G:92:MET:HA	2.21	0.41
1:A:135:GLN:CG	1:A:185:THR:HG21	2.51	0.41
1:G:44:ARG:HH22	1:H:51:GLU:CD	2.23	0.41
1:C:180:THR:HG21	1:C:199:ILE:HD13	2.02	0.41
1:F:187:LYS:HG3	1:F:187:LYS:HZ3	1.78	0.41
1:G:133:SER:O	1:G:184:VAL:HG22	2.21	0.41
1:H:124:LEU:HD23	1:H:215:PHE:CE1	2.56	0.41
1:H:94:ARG:HB3	2:H:217:T5A:HB72	2.03	0.41
1:B:65:ILE:HG23	1:B:66:HIS:N	2.36	0.41
1:A:79:LYS:HD3	3:A:4814:HOH:O	2.21	0.41
1:A:2:MET:O	1:A:207:HIS:CE1	2.74	0.40
1:E:154:VAL:O	1:E:158:GLU:HB2	2.21	0.40
1:C:3:GLY:O	1:C:210:HIS:CE1	2.75	0.40
1:G:143:LYS:HG3	1:G:145:GLY:CA	2.51	0.40
1:H:56:ASP:OD1	1:H:56:ASP:C	2.60	0.40
1:C:18:LYS:HB2	1:C:18:LYS:HE2	1.88	0.40
1:D:134:THR:HG22	3:D:4962:HOH:O	2.20	0.40
1:C:169:ASP:O	1:C:172:ILE:HB	2.21	0.40
1:D:12:GLY:HA2	1:D:131:PHE:CE1	2.56	0.40
1:E:185:THR:O	1:E:186:ASN:HB2	2.21	0.40
1:H:33:CYS:HA	1:H:89:ASN:O	2.21	0.40
1:F:173:ARG:NE	3:F:4660:HOH:O	2.31	0.40
1:D:82:LYS:HE2	1:D:86:GLU:OE2	2.22	0.40
1:D:26:TYR:O	1:D:30:GLN:HG3	2.20	0.40
3:B:4313:HOH:O	1:E:190:GLN:HB3	2.21	0.40
1:B:71:ALA:O	1:B:75:GLU:HG2	2.22	0.40
1:C:81:LYS:HG2	1:C:124:LEU:HD11	2.02	0.40
1:E:215:PHE:N	1:E:215:PHE:CD1	2.89	0.40
1:H:111:MET:HG2	1:H:115:TRP:CZ3	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:OE2	1:F:191:GLU:OE2[1_556]	2.11	0.09

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	214/216 (99%)	194 (91%)	16 (8%)	4 (2%)	10 4
1	B	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	14 6
1	C	201/216 (93%)	191 (95%)	8 (4%)	2 (1%)	19 11
1	D	212/216 (98%)	205 (97%)	6 (3%)	1 (0%)	34 26
1	E	213/216 (99%)	196 (92%)	11 (5%)	6 (3%)	6 2
1	F	214/216 (99%)	204 (95%)	8 (4%)	2 (1%)	21 13
1	G	213/216 (99%)	193 (91%)	14 (7%)	6 (3%)	6 2
1	H	212/216 (98%)	198 (93%)	11 (5%)	3 (1%)	14 6
All	All	1693/1728 (98%)	1582 (93%)	84 (5%)	27 (2%)	12 5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	VAL
1	G	142	GLU
1	G	145	GLY
1	G	146	PHE
1	G	148	ASP
1	H	142	GLU
1	A	147	GLY
1	B	209	ASP
1	B	210	HIS
1	C	152	GLU
1	E	145	GLY
1	E	146	PHE
1	E	148	ASP
1	H	144	SER
1	A	210	HIS
1	E	210	HIS
1	H	143	LYS

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Mol	Chain	Res	Type
1	B	95	TYR
1	C	95	TYR
1	D	95	TYR
1	F	95	TYR
1	F	141	ALA
1	G	139	ASN
1	G	141	ALA
1	A	148	ASP
1	E	95	TYR
1	E	144	SER

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	194/194 (100%)	171 (88%)	23 (12%)	6 3
1	B	193/194 (100%)	175 (91%)	18 (9%)	11 6
1	C	186/194 (96%)	158 (85%)	28 (15%)	3 1
1	D	188/194 (97%)	172 (92%)	16 (8%)	13 8
1	E	192/194 (99%)	169 (88%)	23 (12%)	6 3
1	F	192/194 (99%)	173 (90%)	19 (10%)	10 5
1	G	192/194 (99%)	171 (89%)	21 (11%)	8 4
1	H	188/194 (97%)	173 (92%)	15 (8%)	15 9
All	All	1525/1552 (98%)	1362 (89%)	163 (11%)	8 4

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	40	GLU
1	A	44	ARG
1	A	76	ILE
1	A	88	LYS

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Mol	Chain	Res	Type
1	A	98	SER
1	A	114	ASP
1	A	130	LEU
1	A	135	GLN
1	A	142	GLU
1	A	143	LYS
1	A	146	PHE
1	A	148	ASP
1	A	153	THR
1	A	162	GLN
1	A	164	PHE
1	A	165	MET
1	A	166	LYS
1	A	171	GLU
1	A	172	ILE
1	A	173	ARG
1	A	212	LYS
1	A	214	SER
1	B	28	LYS
1	B	40	GLU
1	B	59	GLN
1	B	79	LYS
1	B	98	SER
1	B	109	ASN
1	B	125	LYS
1	B	139	ASN
1	B	140	ASN
1	B	142	GLU
1	B	155	LYS
1	B	161	LYS
1	B	164	PHE
1	B	170	LYS
1	B	205	SER
1	B	207	HIS
1	B	209	ASP
1	B	212	LYS
1	C	1	MET
1	C	2	MET
1	C	28	LYS
1	C	34	LYS
1	C	40	GLU
1	C	42	SER

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Mol	Chain	Res	Type
1	C	44	ARG
1	C	81	LYS
1	C	98	SER
1	C	114	ASP
1	C	130	LEU
1	C	136	ASP
1	C	148	ASP
1	C	153	THR
1	C	154	VAL
1	C	159	LYS
1	C	162	GLN
1	C	163	THR
1	C	164	PHE
1	C	170	LYS
1	C	171	GLU
1	C	172	ILE
1	C	174	LYS
1	C	177	GLU
1	C	181	ILE
1	C	187	LYS
1	C	204	LEU
1	C	212	LYS
1	D	28	LYS
1	D	40	GLU
1	D	44	ARG
1	D	79	LYS
1	D	98	SER
1	D	109	ASN
1	D	125	LYS
1	D	135	GLN
1	D	143	LYS
1	D	158	GLU
1	D	164	PHE
1	D	181	ILE
1	D	190	GLN
1	D	206	THR
1	D	207	HIS
1	D	214	SER
1	E	2	MET
1	E	34	LYS
1	E	40	GLU
1	E	59	GLN

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Mol	Chain	Res	Type
1	E	60	LEU
1	E	82	LYS
1	E	98	SER
1	E	114	ASP
1	E	130	LEU
1	E	140	ASN
1	E	143	LYS
1	E	148	ASP
1	E	155	LYS
1	E	158	GLU
1	E	161	LYS
1	E	162	GLN
1	E	164	PHE
1	E	165	MET
1	E	166	LYS
1	E	171	GLU
1	E	172	ILE
1	E	173	ARG
1	E	212	LYS
1	F	6	LYS
1	F	28	LYS
1	F	40	GLU
1	F	44	ARG
1	F	59	GLN
1	F	79	LYS
1	F	98	SER
1	F	125	LYS
1	F	135	GLN
1	F	137	VAL
1	F	138	ASP
1	F	143	LYS
1	F	158	GLU
1	F	161	LYS
1	F	164	PHE
1	F	170	LYS
1	F	205	SER
1	F	211	ASP
1	F	212	LYS
1	G	28	LYS
1	G	34	LYS
1	G	40	GLU
1	G	42	SER

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Mol	Chain	Res	Type
1	G	44	ARG
1	G	98	SER
1	G	114	ASP
1	G	130	LEU
1	G	135	GLN
1	G	140	ASN
1	G	143	LYS
1	G	148	ASP
1	G	158	GLU
1	G	162	GLN
1	G	164	PHE
1	G	165	MET
1	G	166	LYS
1	G	171	GLU
1	G	173	ARG
1	G	174	LYS
1	G	177	GLU
1	H	10	ILE
1	H	28	LYS
1	H	40	GLU
1	H	44	ARG
1	H	79	LYS
1	H	98	SER
1	H	125	LYS
1	H	130	LEU
1	H	144	SER
1	H	155	LYS
1	H	161	LYS
1	H	164	PHE
1	H	170	LYS
1	H	207	HIS
1	H	208	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	162	GLN
1	A	186	ASN
1	A	207	HIS
1	B	32	ASN
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	140	ASN
1	B	207	HIS
1	C	162	GLN
1	C	207	HIS
1	C	210	HIS
1	D	21	GLN
1	D	23	ASN
1	D	32	ASN
1	D	140	ASN
1	D	190	GLN
1	E	59	GLN
1	E	140	ASN
1	E	162	GLN
1	E	186	ASN
1	F	23	ASN
1	F	32	ASN
1	G	162	GLN
1	G	210	HIS
1	H	32	ASN
1	H	109	ASN
1	H	140	ASN

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

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	T5A	A	217	-	41,59,59	1.19	2 (4%)	55,93,93	2.73	8 (14%)
2	T5A	B	217	-	41,59,59	1.43	7 (17%)	55,93,93	2.58	9 (16%)
2	T5A	C	217	-	41,59,59	1.27	4 (9%)	55,93,93	2.95	11 (20%)
2	T5A	D	217	-	41,59,59	1.24	4 (9%)	55,93,93	2.27	9 (16%)
2	T5A	E	217	-	41,59,59	1.39	4 (9%)	55,93,93	2.91	13 (23%)
2	T5A	F	217	-	41,59,59	1.27	6 (14%)	55,93,93	2.45	11 (20%)
2	T5A	G	217	-	41,59,59	1.46	7 (17%)	55,93,93	2.86	8 (14%)
2	T5A	H	217	-	41,59,59	1.50	4 (9%)	55,93,93	2.83	17 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	T5A	A	217	-	-	0/36/72/72	0/5/5/5
2	T5A	B	217	-	-	0/36/72/72	0/5/5/5
2	T5A	C	217	-	-	0/36/72/72	0/5/5/5
2	T5A	D	217	-	-	0/36/72/72	0/5/5/5
2	T5A	E	217	-	-	0/36/72/72	0/5/5/5
2	T5A	F	217	-	-	0/36/72/72	0/5/5/5
2	T5A	G	217	-	-	0/36/72/72	0/5/5/5
2	T5A	H	217	-	-	0/36/72/72	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	217	T5A	C8A-N7A	-2.96	1.28	1.34
2	F	217	T5A	C6B-C5B	-2.77	1.32	1.40
2	B	217	T5A	C6B-C5B	-2.74	1.32	1.40
2	H	217	T5A	C6B-C5B	-2.73	1.32	1.40
2	G	217	T5A	PD-O1D	-2.64	1.43	1.54
2	G	217	T5A	C8A-N7A	-2.55	1.29	1.34
2	E	217	T5A	C6B-C5B	-2.49	1.33	1.40
2	C	217	T5A	PB-O2X	-2.41	1.44	1.54
2	F	217	T5A	C8A-N7A	-2.37	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	T5A	C8A-N7A	-2.34	1.30	1.34
2	D	217	T5A	C6B-C5B	-2.24	1.34	1.40
2	F	217	T5A	O4B-C4B	-2.17	1.19	1.24
2	G	217	T5A	C6B-C5B	-2.17	1.34	1.40
2	C	217	T5A	C6B-C5B	-2.14	1.34	1.40
2	D	217	T5A	PB-O2X	-2.01	1.46	1.54
2	B	217	T5A	C2A-N3A	2.08	1.35	1.32
2	B	217	T5A	C5F-C4F	2.12	1.58	1.51
2	F	217	T5A	O3F-C3F	2.16	1.48	1.43
2	B	217	T5A	C4B-N3B	2.19	1.37	1.33
2	D	217	T5A	C4A-N3A	2.24	1.38	1.35
2	B	217	T5A	C6B-N1B	2.28	1.38	1.35
2	F	217	T5A	C2A-N3A	2.37	1.36	1.32
2	H	217	T5A	C2A-N3A	2.46	1.36	1.32
2	A	217	T5A	O4F-C1F	2.50	1.44	1.41
2	G	217	T5A	C4A-N3A	2.52	1.39	1.35
2	E	217	T5A	O3F-C3F	2.73	1.49	1.43
2	A	217	T5A	C4B-N3B	2.82	1.38	1.33
2	G	217	T5A	C4B-N3B	2.89	1.38	1.33
2	C	217	T5A	O4F-C1F	2.91	1.44	1.41
2	H	217	T5A	C2E-C1E	2.98	1.60	1.52
2	G	217	T5A	O4F-C1F	3.06	1.45	1.41
2	D	217	T5A	O4F-C1F	3.12	1.45	1.41
2	F	217	T5A	O4F-C1F	3.20	1.45	1.41
2	G	217	T5A	C2A-N3A	3.25	1.37	1.32
2	C	217	T5A	C4B-N3B	3.75	1.40	1.33
2	B	217	T5A	O4F-C1F	4.02	1.46	1.41
2	E	217	T5A	O4F-C1F	4.54	1.46	1.41
2	H	217	T5A	O4F-C1F	5.61	1.48	1.41

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	217	T5A	C5B-C4B-N3B	-11.98	111.80	125.14
2	G	217	T5A	C5B-C4B-N3B	-11.76	112.04	125.14
2	E	217	T5A	C5B-C4B-N3B	-11.39	112.45	125.14
2	A	217	T5A	C5B-C4B-N3B	-10.83	113.08	125.14
2	H	217	T5A	C5B-C4B-N3B	-10.64	113.29	125.14
2	B	217	T5A	C5B-C4B-N3B	-9.88	114.14	125.14
2	D	217	T5A	C5B-C4B-N3B	-8.10	116.12	125.14
2	F	217	T5A	C5B-C4B-N3B	-8.01	116.22	125.14
2	H	217	T5A	O3D-PE-O5F	-4.07	92.13	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	217	T5A	O4E-C1E-C2E	-4.01	98.28	106.27
2	C	217	T5A	O3D-PE-O5F	-3.94	92.48	102.94
2	B	217	T5A	C4E-O4E-C1E	-3.83	99.80	109.47
2	E	217	T5A	O4E-C1E-C2E	-3.78	98.74	106.27
2	F	217	T5A	C4E-O4E-C1E	-3.71	100.08	109.47
2	H	217	T5A	C4E-O4E-C1E	-3.65	100.25	109.47
2	D	217	T5A	C4E-O4E-C1E	-3.44	100.78	109.47
2	E	217	T5A	C4F-O4F-C1F	-3.42	105.97	109.72
2	D	217	T5A	C1F-N9A-C4A	-3.38	121.84	126.94
2	A	217	T5A	C4E-O4E-C1E	-3.38	100.93	109.47
2	B	217	T5A	C2F-C1F-N9A	-2.96	109.77	114.29
2	H	217	T5A	C2F-C3F-C4F	-2.92	96.61	102.61
2	C	217	T5A	C4E-O4E-C1E	-2.88	102.20	109.47
2	H	217	T5A	O4E-C1E-C2E	-2.84	100.60	106.27
2	A	217	T5A	O4E-C1E-C2E	-2.84	100.61	106.27
2	G	217	T5A	C4E-O4E-C1E	-2.79	102.41	109.47
2	E	217	T5A	C2F-C3F-C4F	-2.76	96.94	102.61
2	G	217	T5A	O3D-PE-O5F	-2.66	95.89	102.94
2	B	217	T5A	O4E-C1E-C2E	-2.64	101.00	106.27
2	E	217	T5A	O3E-C3E-C2E	-2.64	101.99	110.74
2	C	217	T5A	N3A-C2A-N1A	-2.64	126.87	128.89
2	G	217	T5A	O3E-C3E-C2E	-2.58	102.19	110.74
2	H	217	T5A	C1F-N9A-C4A	-2.55	123.09	126.94
2	A	217	T5A	O3F-C3F-C4F	-2.54	103.44	111.05
2	D	217	T5A	O3F-C3F-C4F	-2.47	103.64	111.05
2	F	217	T5A	C2F-C3F-C4F	-2.46	97.56	102.61
2	B	217	T5A	O3D-PE-O5F	-2.45	96.43	102.94
2	F	217	T5A	O3A-PA-O5E	-2.43	96.49	102.94
2	E	217	T5A	O3D-PE-O5F	-2.30	96.82	102.94
2	B	217	T5A	C2F-C3F-C4F	-2.25	97.99	102.61
2	A	217	T5A	O3D-PE-O5F	-2.23	97.02	102.94
2	H	217	T5A	O3A-PA-O5E	-2.22	97.05	102.94
2	H	217	T5A	C4F-O4F-C1F	-2.06	107.46	109.72
2	H	217	T5A	O1D-PD-O3C	2.01	114.19	105.09
2	G	217	T5A	O2C-PC-O3B	2.04	114.37	105.09
2	B	217	T5A	O4F-C1F-N9A	2.05	112.38	108.10
2	F	217	T5A	O1D-PD-O3C	2.06	114.42	105.09
2	F	217	T5A	O4F-C1F-N9A	2.06	112.40	108.10
2	E	217	T5A	O2C-PC-O3B	2.07	114.48	105.09
2	E	217	T5A	O1D-PD-O3C	2.10	114.63	105.09
2	F	217	T5A	PC-O3B-PB	2.10	138.63	132.73
2	E	217	T5A	O1D-PD-O2D	2.11	123.99	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	217	T5A	O1A-PA-O5E	2.12	119.14	108.46
2	H	217	T5A	PC-O3B-PB	2.15	138.76	132.73
2	G	217	T5A	O2X-PB-O1B	2.28	124.88	112.53
2	E	217	T5A	O4F-C1F-N9A	2.36	113.04	108.10
2	F	217	T5A	O2X-PB-O1B	2.39	125.46	112.53
2	F	217	T5A	O1E-PE-O5F	2.41	120.61	108.46
2	H	217	T5A	O2C-PC-O1C	2.42	125.62	112.53
2	C	217	T5A	O2X-PB-O3B	2.42	116.06	105.09
2	H	217	T5A	O2X-PB-O1B	2.44	125.72	112.53
2	C	217	T5A	O4F-C1F-N9A	2.44	113.20	108.10
2	H	217	T5A	O2F-C2F-C3F	2.54	120.08	111.83
2	H	217	T5A	O4F-C1F-N9A	2.57	113.48	108.10
2	F	217	T5A	O2C-PC-O1C	2.63	126.78	112.53
2	H	217	T5A	O4E-C4E-C3E	2.64	112.30	105.67
2	A	217	T5A	O2C-PC-O3B	2.64	117.08	105.09
2	D	217	T5A	O2C-PC-O1C	2.66	126.93	112.53
2	C	217	T5A	PC-O3B-PB	2.72	140.36	132.73
2	D	217	T5A	C2F-C1F-N9A	2.75	118.50	114.29
2	B	217	T5A	O2X-PB-O1B	2.76	127.50	112.53
2	C	217	T5A	O1D-PD-O2D	2.79	127.64	112.53
2	A	217	T5A	PC-O3B-PB	2.82	140.64	132.73
2	D	217	T5A	O2X-PB-O1B	2.83	127.89	112.53
2	H	217	T5A	O4E-C1E-N1B	2.93	112.78	107.72
2	G	217	T5A	PC-O3B-PB	2.93	140.96	132.73
2	E	217	T5A	O4E-C1E-N1B	2.96	112.84	107.72
2	D	217	T5A	O4F-C1F-N9A	3.05	114.48	108.10
2	E	217	T5A	PC-O3B-PB	3.07	141.36	132.73
2	D	217	T5A	C4B-N3B-C2B	10.51	124.33	115.25
2	F	217	T5A	C4B-N3B-C2B	12.44	126.00	115.25
2	B	217	T5A	C4B-N3B-C2B	12.86	126.36	115.25
2	H	217	T5A	C4B-N3B-C2B	13.08	126.56	115.25
2	A	217	T5A	C4B-N3B-C2B	14.15	127.48	115.25
2	E	217	T5A	C4B-N3B-C2B	14.52	127.80	115.25
2	G	217	T5A	C4B-N3B-C2B	14.86	128.09	115.25
2	C	217	T5A	C4B-N3B-C2B	14.90	128.13	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	217	T5A	1	0
2	B	217	T5A	1	0
2	C	217	T5A	3	0
2	E	217	T5A	1	0
2	H	217	T5A	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	216/216 (100%)	0.11	14 (6%)	22	23	8, 19, 42, 56	0
1	B	216/216 (100%)	-0.14	5 (2%)	64	64	8, 17, 42, 49	0
1	C	205/216 (94%)	0.01	4 (1%)	68	69	8, 18, 38, 49	0
1	D	214/216 (99%)	-0.15	5 (2%)	64	64	8, 17, 36, 46	0
1	E	215/216 (99%)	0.10	13 (6%)	25	27	7, 20, 45, 49	0
1	F	216/216 (100%)	-0.14	5 (2%)	64	64	8, 17, 36, 49	0
1	G	215/216 (99%)	-0.01	8 (3%)	45	47	7, 19, 41, 47	0
1	H	214/216 (99%)	-0.05	8 (3%)	45	47	7, 17, 41, 50	0
All	All	1711/1728 (99%)	-0.03	62 (3%)	46	48	7, 18, 41, 56	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	8.0
1	A	2	MET	5.6
1	E	2	MET	5.5
1	G	146	PHE	5.0
1	A	1	MET	4.9
1	F	141	ALA	4.4
1	H	211	ASP	4.2
1	A	147	GLY	4.1
1	A	146	PHE	3.8
1	C	153	THR	3.8
1	E	141	ALA	3.8
1	G	145	GLY	3.7
1	A	137	VAL	3.6
1	H	141	ALA	3.6
1	B	141	ALA	3.5
1	D	210	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	210	HIS	3.4
1	B	208	ILE	3.4
1	A	144	SER	3.3
1	A	3	GLY	3.2
1	G	147	GLY	3.2
1	E	147	GLY	3.1
1	C	152	GLU	3.0
1	A	145	GLY	3.0
1	E	208	ILE	3.0
1	B	137	VAL	3.0
1	C	154	VAL	3.0
1	E	210	HIS	2.9
1	G	173	ARG	2.9
1	E	3	GLY	2.9
1	G	140	ASN	2.9
1	A	139	ASN	2.9
1	D	3	GLY	2.8
1	F	140	ASN	2.7
1	F	137	VAL	2.7
1	H	137	VAL	2.7
1	D	208	ILE	2.6
1	E	145	GLY	2.6
1	E	146	PHE	2.5
1	G	144	SER	2.4
1	H	3	GLY	2.4
1	A	141	ALA	2.4
1	H	144	SER	2.4
1	H	143	LYS	2.2
1	G	139	ASN	2.2
1	A	148	ASP	2.2
1	F	142	GLU	2.1
1	D	137	VAL	2.1
1	A	206	THR	2.1
1	B	139	ASN	2.1
1	D	211	ASP	2.1
1	E	148	ASP	2.1
1	E	173	ARG	2.1
1	A	135	GLN	2.0
1	F	143	LYS	2.0
1	E	139	ASN	2.0
1	E	142	GLU	2.0
1	E	211	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	148	ASP	2.0
1	A	208	ILE	2.0
1	B	209	ASP	2.0
1	H	209	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	T5A	F	217	55/55	0.97	0.11	-0.06	3,18,28,29	0
2	T5A	B	217	55/55	0.98	0.10	-0.09	7,16,25,26	0
2	T5A	A	217	55/55	0.98	0.10	-0.42	7,15,26,28	0
2	T5A	C	217	55/55	0.98	0.10	-0.44	6,14,26,27	0
2	T5A	E	217	55/55	0.98	0.10	-0.47	4,15,27,28	0
2	T5A	H	217	55/55	0.98	0.09	-0.52	2,16,25,26	0
2	T5A	D	217	55/55	0.98	0.10	-0.65	2,13,24,26	0
2	T5A	G	217	55/55	0.98	0.10	-0.66	4,12,23,26	0

6.5 Other polymers (i)

There are no such residues in this entry.