



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:07 PM GMT

PDB ID : 2J4K
Title : CRYSTAL STRUCTURE OF URIDYLATE KINASE FROM SULFOLOBUS SOLFATARICUS IN COMPLEX WITH UMP TO 2.2 ANGSTROM RESOLUTION
Authors : Jensen, K.S.; Johansson, E.; Jensen, K.F.
Deposited on : 2006-09-01
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

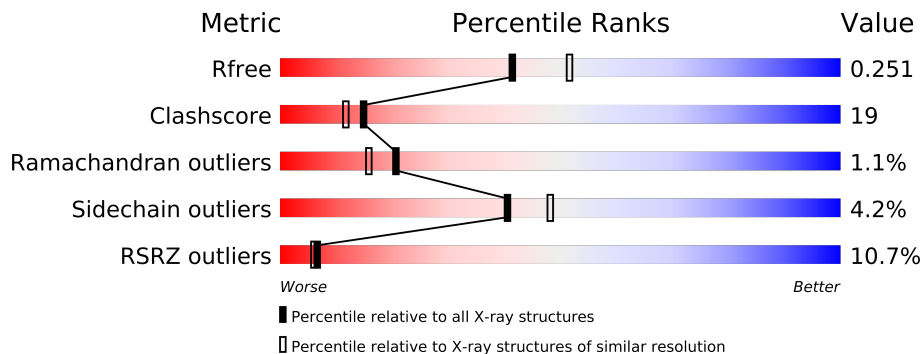
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	
1	F	226	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	U5P	B	227	-	X
2	U5P	C	227	-	X
4	MG	A	231	-	X

2 Entry composition i

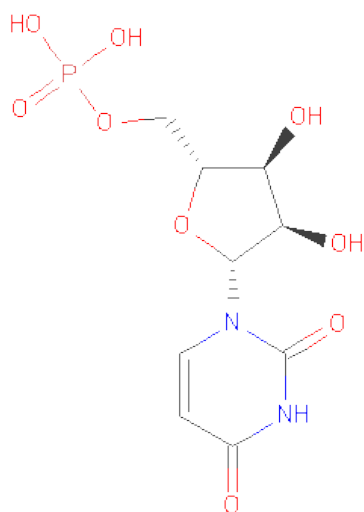
There are 5 unique types of molecules in this entry. The entry contains 10413 atoms, of which 0 are hydrogen and 0 are deuterium.

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 URIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1620	1040	278	298	4			
1	B	214	Total	C	N	O	S	0	0	0
			1675	1074	286	311	4			
1	C	206	Total	C	N	O	S	0	0	0
			1612	1033	276	299	4			
1	D	226	Total	C	N	O	S	0	0	0
			1761	1126	300	331	4			
1	E	221	Total	C	N	O	S	0	0	0
			1722	1101	294	323	4			
1	F	208	Total	C	N	O	S	0	0	0
			1619	1039	276	300	4			

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	E	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	F	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cd	0	0
			1	1		
3	E	2	Total	Cd	0	0
			2	2		
3	B	7	Total	Cd	0	0
			7	7		
3	C	3	Total	Cd	0	0
			3	3		
3	A	3	Total	Cd	0	0
			3	3		
3	F	2	Total	Cd	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		
5	B	49	Total	O	0	0
			49	49		

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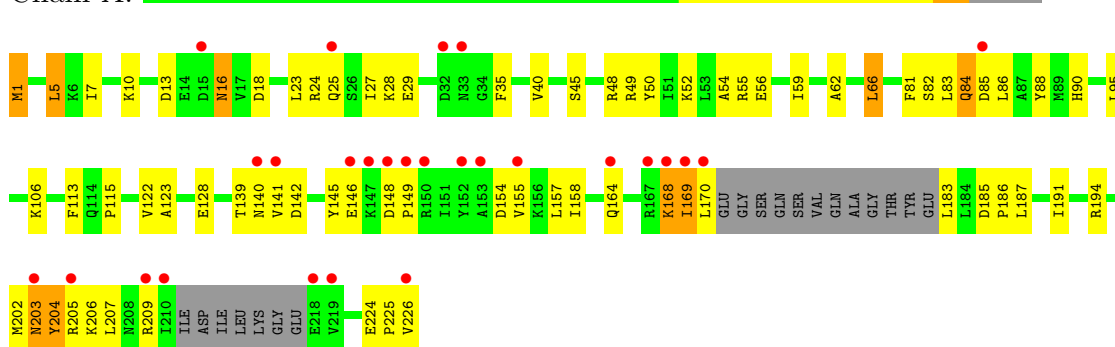
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	25	Total 25	O 25	0	0
5	D	51	Total 51	O 51	0	0
5	E	50	Total 50	O 50	0	0
5	F	44	Total 44	O 44	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

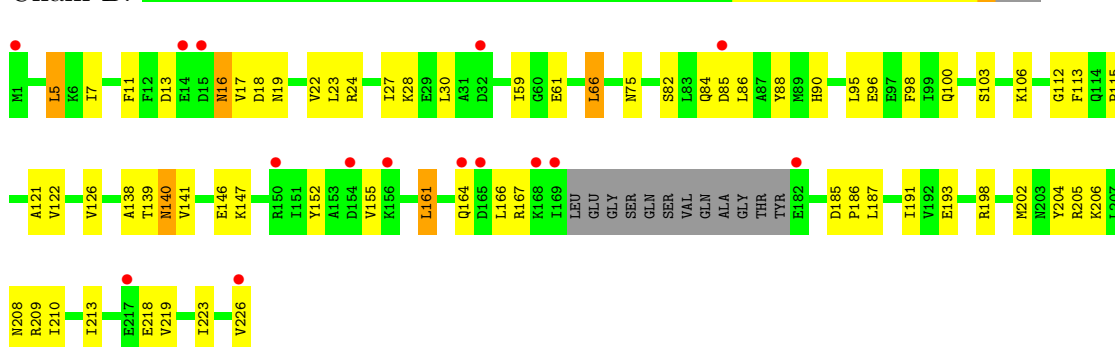
• Molecule 1: URIDYLATE KINASE

Chain A:



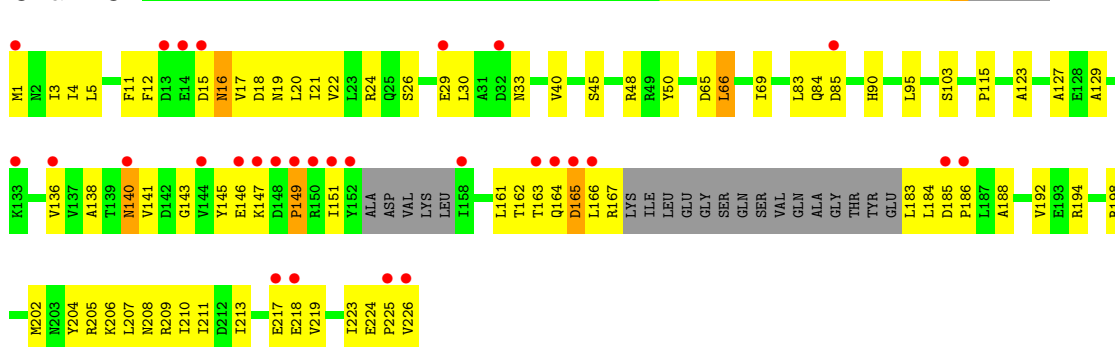
• Molecule 1: URIDYLATE KINASE

Chain B:



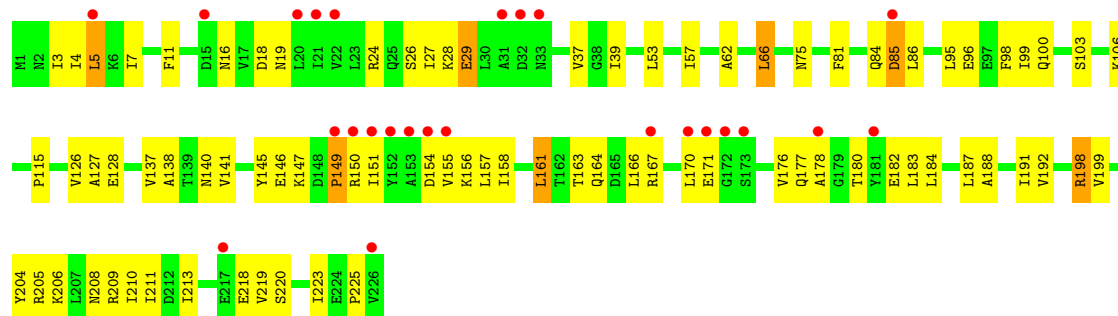
• Molecule 1: URIDYLATE KINASE

Chain C:



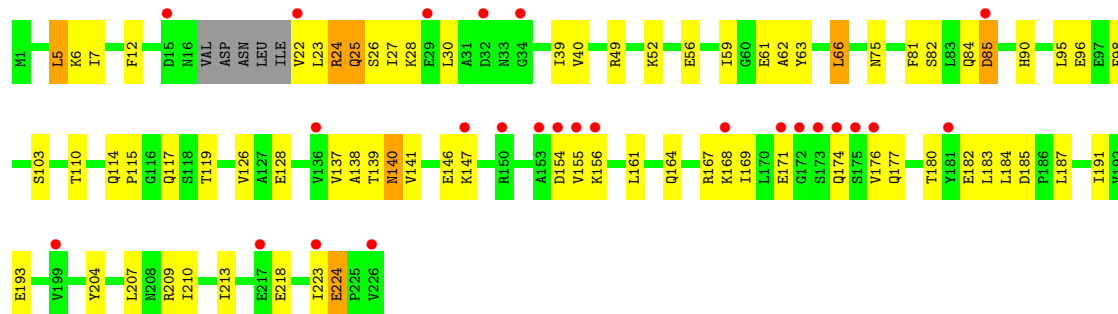
• Molecule 1: URIDYLATE KINASE

Chain D: 



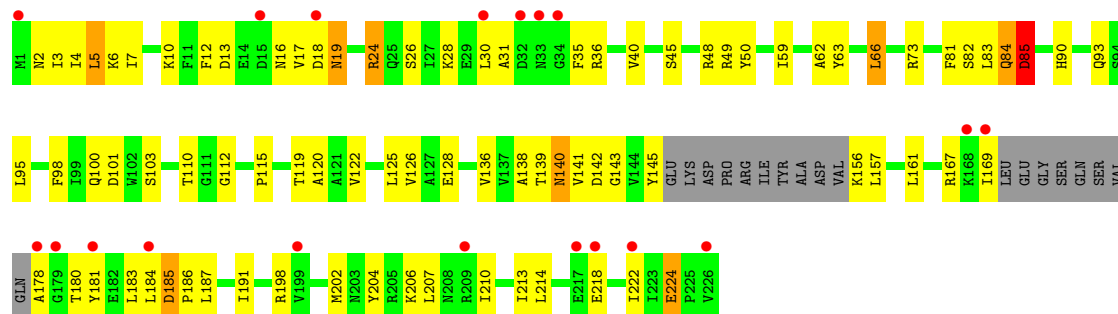
• Molecule 1: URIDYLATE KINASE

Chain E: 



• Molecule 1: URIDYLATE KINASE

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.80Å 136.04Å 77.94Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	21.67 – 2.20 21.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (21.67-2.20) 99.1 (21.67-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.251 0.219 , 0.251	Depositor DCC
R_{free} test set	3363 reflections (4.68%)	DCC
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 43.0	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 71828 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10413	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, U5P, CD

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	0.33	0/1643	0.61	0/2220
1	B	0.33	0/1699	0.62	0/2296
1	C	0.33	0/1635	0.62	0/2209
1	D	0.34	0/1787	0.61	0/2417
1	E	0.33	0/1747	0.62	0/2360
1	F	0.35	0/1641	0.63	0/2216
All	All	0.33	0/10152	0.62	0/13718

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1620	0	1687	78	0
1	B	1675	0	1742	68	0
1	C	1612	0	1669	68	0
1	D	1761	0	1822	76	0
1	E	1722	0	1780	72	0
1	F	1619	0	1684	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	21	0	11	0	0
2	B	21	0	11	1	0
2	C	21	0	11	0	0
2	D	21	0	11	0	0
2	E	21	0	11	0	0
2	F	21	0	11	0	0
3	A	3	0	0	0	0
3	B	7	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
5	A	40	0	0	6	0
5	B	49	0	0	2	0
5	C	25	0	0	1	0
5	D	51	0	0	2	0
5	E	50	0	0	3	0
5	F	44	0	0	2	0
All	All	10413	0	10450	394	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (394) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:145:TYR:H	1:D:177:GLN:HE22	1.00	0.98
1:D:137:VAL:HG21	1:D:183:LEU:HD21	1.44	0.97
1:C:146:GLU:HG3	1:C:147:LYS:HG2	1.43	0.97
1:B:30:LEU:HD21	1:B:210:ILE:HD13	1.48	0.95
1:B:185:ASP:HB2	1:B:186:PRO:HD2	1.50	0.93
1:A:139:THR:HG22	1:A:140:ASN:H	1.33	0.92
1:A:185:ASP:HB2	1:A:186:PRO:HD2	1.56	0.88
1:D:164:GLN:HA	1:D:167:ARG:HE	1.41	0.85
1:D:198:ARG:HB3	1:D:198:ARG:HH11	1.44	0.83
1:A:203:ASN:HB2	5:A:2036:HOH:O	1.80	0.80
1:A:207:LEU:HA	5:A:2037:HOH:O	1.81	0.79
1:F:181:TYR:HA	1:F:184:LEU:HD12	1.64	0.78
1:E:176:VAL:HG12	1:E:177:GLN:H	1.48	0.78
1:A:115:PRO:HG2	1:E:95:LEU:HD23	1.65	0.78
1:F:198:ARG:HH21	1:F:222:ILE:HG21	1.50	0.77
1:E:213:ILE:HD13	1:E:218:GLU:HB3	1.66	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:24:ARG:HH11	1:F:28:LYS:HE3	1.50	0.76
1:A:139:THR:HG22	1:A:140:ASN:N	2.01	0.76
1:C:162:THR:OG1	1:C:165:ASP:HB2	1.85	0.76
1:B:164:GLN:HG3	1:B:226:VAL:CG2	2.16	0.76
1:F:84:GLN:O	1:F:85:ASP:HB2	1.87	0.75
1:B:206:LYS:HG2	1:B:209:ARG:HH21	1.52	0.74
1:D:176:VAL:HG22	1:D:177:GLN:H	1.52	0.74
1:C:164:GLN:HG3	1:C:226:VAL:HG23	1.69	0.74
1:B:164:GLN:HG3	1:B:226:VAL:HG23	1.70	0.73
1:E:146:GLU:OE1	1:E:156:LYS:HE3	1.89	0.72
1:C:207:LEU:HD22	1:C:210:ILE:HD11	1.72	0.71
1:E:59:ILE:HD11	1:F:82:SER:HA	1.73	0.71
1:D:26:SER:O	1:D:29:GLU:HB2	1.91	0.70
1:C:185:ASP:HB2	1:C:186:PRO:HD2	1.74	0.70
1:B:28:LYS:HG2	1:B:86:LEU:HD11	1.74	0.70
1:D:145:TYR:N	1:D:177:GLN:HE22	1.84	0.70
1:B:213:ILE:HD13	1:B:218:GLU:HB3	1.73	0.70
1:E:52:LYS:O	1:E:56:GLU:HG3	1.92	0.70
1:F:10:LYS:HD3	1:F:140:ASN:OD1	1.93	0.69
1:C:207:LEU:O	1:C:210:ILE:HG13	1.93	0.68
1:D:84:GLN:O	1:D:85:ASP:HB2	1.91	0.68
1:B:84:GLN:O	1:B:85:ASP:HB2	1.93	0.68
1:E:147:LYS:HB2	1:E:155:VAL:HG11	1.77	0.67
1:C:11:PHE:CE1	1:C:19:ASN:HB3	2.31	0.66
1:B:66:LEU:HD13	1:B:115:PRO:HG3	1.76	0.66
1:C:138:ALA:HB1	1:C:204:TYR:HB3	1.78	0.66
1:B:209:ARG:O	1:B:213:ILE:HG12	1.96	0.66
1:B:166:LEU:HD22	1:B:223:ILE:HD13	1.76	0.66
1:D:167:ARG:O	1:D:171:GLU:HG3	1.96	0.65
1:E:164:GLN:O	1:E:168:LYS:HG2	1.97	0.65
1:B:61:GLU:HG2	1:C:194:ARG:HD2	1.79	0.65
1:B:96:GLU:HG3	5:C:2017:HOH:O	1.96	0.65
1:D:62:ALA:HB2	1:F:128:GLU:HG2	1.77	0.65
1:A:187:LEU:O	1:A:191:ILE:HG12	1.97	0.65
1:E:176:VAL:O	1:E:177:GLN:HG3	1.98	0.64
1:B:95:LEU:HD23	1:C:115:PRO:HG2	1.80	0.64
1:D:96:GLU:HG3	5:F:2026:HOH:O	1.97	0.64
1:A:95:LEU:HD23	1:E:115:PRO:HG2	1.80	0.63
1:C:20:LEU:HD13	1:D:57:ILE:HD13	1.79	0.63
1:A:139:THR:CG2	1:A:140:ASN:H	2.09	0.63
1:A:84:GLN:O	1:A:85:ASP:HB2	1.98	0.63
1:D:145:TYR:H	1:D:177:GLN:NE2	1.84	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:188:ALA:O	1:C:192:VAL:HG13	1.99	0.62
1:F:24:ARG:NH1	1:F:28:LYS:HE3	2.12	0.62
1:F:138:ALA:HB1	1:F:204:TYR:HB3	1.82	0.62
1:D:141:VAL:HG21	1:D:178:ALA:O	2.00	0.62
1:B:138:ALA:HB1	1:B:204:TYR:HB3	1.81	0.61
1:E:224:GLU:HG3	5:E:2048:HOH:O	2.01	0.61
1:E:169:ILE:CD1	1:E:180:THR:HG21	2.31	0.61
1:A:168:LYS:HA	1:A:168:LYS:HE3	1.81	0.61
1:B:98:PHE:CZ	1:B:126:VAL:HG13	2.35	0.61
1:D:164:GLN:HA	1:D:167:ARG:NE	2.13	0.61
1:D:81:PHE:O	1:D:84:GLN:HG3	2.01	0.61
1:D:176:VAL:HG22	1:D:177:GLN:N	2.14	0.60
1:D:161:LEU:N	1:D:161:LEU:HD23	2.16	0.60
1:A:141:VAL:HG12	1:A:142:ASP:N	2.16	0.60
1:A:203:ASN:HD21	1:A:206:LYS:CG	2.15	0.60
1:D:198:ARG:CB	1:D:198:ARG:HH11	2.13	0.60
1:A:16:ASN:HD22	1:A:18:ASP:H	1.50	0.60
1:E:176:VAL:HG12	1:E:177:GLN:N	2.16	0.59
1:D:100:GLN:O	1:D:103:SER:HB3	2.02	0.59
1:D:206:LYS:HG2	1:D:209:ARG:HH21	1.67	0.59
1:F:3:ILE:HD11	1:F:136:VAL:CG2	2.32	0.59
1:E:5:LEU:HD13	1:E:7:ILE:HD11	1.85	0.59
1:C:163:THR:HG23	1:C:225:PRO:HA	1.83	0.58
1:E:169:ILE:HG12	1:E:174:GLN:HB3	1.86	0.58
1:F:210:ILE:O	1:F:214:LEU:HG	2.03	0.58
1:C:164:GLN:NE2	1:C:226:VAL:OXT	2.36	0.58
1:F:45:SER:HA	1:F:48:ARG:NH1	2.18	0.58
1:B:140:ASN:HD22	1:B:141:VAL:N	2.02	0.58
1:F:198:ARG:NH2	1:F:222:ILE:HG21	2.20	0.57
1:C:213:ILE:HD13	1:C:218:GLU:HB3	1.85	0.57
1:B:185:ASP:CB	1:B:186:PRO:HD2	2.29	0.57
1:A:115:PRO:HG2	1:E:95:LEU:CD2	2.35	0.57
1:E:84:GLN:O	1:E:85:ASP:HB2	2.04	0.57
1:C:26:SER:HB2	1:C:210:ILE:HD12	1.86	0.57
1:E:138:ALA:HB1	1:E:204:TYR:HB3	1.87	0.56
1:E:169:ILE:HD13	1:E:180:THR:HG21	1.88	0.56
1:E:169:ILE:CG1	1:E:174:GLN:HB3	2.36	0.56
1:B:18:ASP:O	1:B:22:VAL:HG12	2.05	0.56
1:E:49:ARG:HH22	1:F:13:ASP:HA	1.71	0.56
1:C:17:VAL:O	1:C:21:ILE:HG12	2.04	0.56
1:A:169:ILE:O	1:A:169:ILE:HG22	2.06	0.56
1:A:203:ASN:HD21	1:A:206:LYS:HG3	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:THR:CG2	1:C:225:PRO:HA	2.36	0.56
1:D:28:LYS:HE3	1:D:86:LEU:HD21	1.87	0.56
1:C:26:SER:O	1:C:30:LEU:HD23	2.05	0.56
1:F:180:THR:O	1:F:184:LEU:HG	2.06	0.56
1:B:206:LYS:CG	1:B:209:ARG:HH21	2.17	0.55
1:F:66:LEU:HD13	1:F:115:PRO:HG3	1.86	0.55
1:E:82:SER:HA	1:F:59:ILE:HD11	1.88	0.55
1:D:177:GLN:H	1:D:180:THR:HG22	1.71	0.55
1:B:206:LYS:HG2	1:B:209:ARG:NH2	2.21	0.55
1:E:75:ASN:ND2	1:F:50:TYR:OH	2.40	0.55
1:E:12:PHE:O	1:F:49:ARG:NH2	2.35	0.55
1:E:139:THR:HG23	1:E:141:VAL:H	1.71	0.55
1:E:22:VAL:O	1:E:25:GLN:NE2	2.39	0.55
1:E:207:LEU:O	1:E:210:ILE:HG13	2.07	0.55
1:D:28:LYS:HG2	1:D:86:LEU:HD11	1.89	0.55
1:C:224:GLU:OE2	1:C:225:PRO:HD2	2.07	0.55
1:A:164:GLN:HG3	1:A:226:VAL:CG2	2.37	0.55
1:D:187:LEU:O	1:D:191:ILE:HG12	2.07	0.55
1:B:16:ASN:HD22	1:B:16:ASN:N	2.04	0.54
1:F:2:ASN:OD1	1:F:36:ARG:HB2	2.08	0.54
1:F:48:ARG:NH1	5:F:2010:HOH:O	2.40	0.54
1:A:29:GLU:HB3	1:A:209:ARG:NH2	2.23	0.54
1:A:115:PRO:CG	1:E:95:LEU:HD23	2.36	0.54
1:A:28:LYS:HG2	1:A:86:LEU:HD11	1.89	0.54
1:D:128:GLU:HG2	1:F:62:ALA:HB2	1.89	0.54
1:A:164:GLN:HG3	1:A:226:VAL:HG23	1.88	0.54
1:B:146:GLU:HG2	1:B:155:VAL:HG13	1.89	0.54
1:A:45:SER:HA	1:A:48:ARG:NH1	2.23	0.54
1:D:16:ASN:HD22	1:D:18:ASP:H	1.56	0.54
1:B:140:ASN:ND2	1:B:141:VAL:HG13	2.23	0.54
1:B:100:GLN:O	1:B:103:SER:HB2	2.07	0.54
1:C:208:ASN:OD1	1:C:209:ARG:HG3	2.08	0.53
1:D:66:LEU:HD13	1:D:115:PRO:HG3	1.90	0.53
1:F:26:SER:O	1:F:30:LEU:HB2	2.08	0.53
1:F:141:VAL:HG12	1:F:143:GLY:H	1.73	0.53
1:B:208:ASN:OD1	1:B:209:ARG:HG3	2.09	0.53
1:C:66:LEU:HD13	1:C:115:PRO:HG3	1.89	0.53
1:B:24:ARG:HD3	1:B:82:SER:O	2.08	0.53
1:C:3:ILE:HD11	1:C:136:VAL:CG2	2.38	0.53
1:E:209:ARG:O	1:E:213:ILE:HG12	2.08	0.53
1:C:3:ILE:HD11	1:C:136:VAL:HG23	1.89	0.53
1:D:98:PHE:CZ	1:D:126:VAL:HG13	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:151:ILE:HG22	1:C:151:ILE:O	2.08	0.53
1:C:166:LEU:HD22	1:C:223:ILE:HD13	1.91	0.53
1:F:95:LEU:HD13	1:F:125:LEU:HB3	1.90	0.52
1:F:120:ALA:HB1	1:F:183:LEU:HD12	1.90	0.52
1:E:27:ILE:HD11	1:E:39:ILE:HD11	1.91	0.52
1:F:3:ILE:HD11	1:F:136:VAL:HG23	1.90	0.52
1:B:23:LEU:O	1:B:27:ILE:HG12	2.08	0.52
1:C:33:ASN:OD1	1:C:211:ILE:HD13	2.09	0.52
1:D:177:GLN:O	1:D:180:THR:HG22	2.09	0.52
1:A:81:PHE:O	1:A:84:GLN:HG3	2.10	0.52
1:E:30:LEU:HD21	1:E:210:ILE:CG2	2.40	0.52
1:C:206:LYS:HG2	1:C:209:ARG:HH21	1.74	0.52
1:E:174:GLN:NE2	5:E:2038:HOH:O	2.39	0.52
1:E:167:ARG:CZ	1:E:193:GLU:OE1	2.58	0.52
1:C:140:ASN:HD22	1:C:140:ASN:H	1.58	0.52
1:D:27:ILE:HD11	1:D:39:ILE:HD11	1.91	0.52
1:F:183:LEU:HG	1:F:183:LEU:O	2.10	0.51
1:B:121:ALA:HB1	1:B:187:LEU:HD23	1.92	0.51
1:B:11:PHE:CE1	1:B:19:ASN:HB3	2.45	0.51
1:A:66:LEU:HD13	1:A:115:PRO:HG3	1.91	0.51
1:C:95:LEU:HD11	1:C:129:ALA:HB2	1.91	0.51
1:C:140:ASN:HD22	1:C:140:ASN:N	2.07	0.51
1:C:141:VAL:HG12	1:C:143:GLY:H	1.75	0.51
1:B:206:LYS:HZ3	1:B:219:VAL:HB	1.75	0.51
1:D:4:ILE:HG13	1:D:127:ALA:HA	1.93	0.51
1:C:84:GLN:O	1:C:85:ASP:HB2	2.11	0.51
1:F:187:LEU:O	1:F:191:ILE:HG12	2.10	0.51
1:A:194:ARG:HD2	1:E:61:GLU:HG2	1.93	0.51
1:A:203:ASN:HD22	1:A:203:ASN:N	2.07	0.51
1:B:61:GLU:HG2	1:C:194:ARG:CD	2.41	0.51
1:A:24:ARG:O	1:A:28:LYS:HG3	2.10	0.50
1:B:115:PRO:HG2	1:C:95:LEU:HD23	1.92	0.50
1:B:66:LEU:HD13	1:B:115:PRO:CG	2.41	0.50
1:C:15:ASP:OD1	1:C:18:ASP:HB2	2.11	0.50
1:D:188:ALA:O	1:D:192:VAL:HG13	2.12	0.50
1:E:147:LYS:HB2	1:E:155:VAL:CG1	2.41	0.50
1:D:163:THR:HG23	1:D:225:PRO:HA	1.94	0.50
1:C:33:ASN:HD22	1:C:33:ASN:N	2.08	0.50
1:D:147:LYS:H	1:D:155:VAL:HG11	1.76	0.50
1:A:149:PRO:HG3	1:A:154:ASP:O	2.12	0.49
1:E:176:VAL:HG13	1:E:184:LEU:CD1	2.42	0.49
1:A:168:LYS:C	1:A:170:LEU:H	2.15	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:GLU:HG3	1:A:225:PRO:HD2	1.94	0.49
1:B:16:ASN:ND2	1:B:16:ASN:H	2.10	0.49
1:F:30:LEU:O	1:F:35:PHE:HB2	2.12	0.49
1:B:218:GLU:HG3	1:B:219:VAL:N	2.28	0.49
1:E:6:LYS:HE3	1:E:119:THR:OG1	2.13	0.49
1:D:206:LYS:HG2	1:D:209:ARG:NH2	2.27	0.49
1:A:209:ARG:HG3	5:A:2039:HOH:O	2.13	0.49
1:F:95:LEU:HG	1:F:95:LEU:O	2.13	0.49
1:A:155:VAL:HG23	1:A:155:VAL:O	2.13	0.49
1:E:49:ARG:NH2	1:F:13:ASP:HA	2.28	0.49
1:E:30:LEU:HD21	1:E:210:ILE:HG22	1.94	0.49
1:E:24:ARG:NH1	1:E:28:LYS:HE3	2.28	0.49
1:D:11:PHE:CZ	1:D:19:ASN:HB2	2.48	0.49
1:E:140:ASN:HD22	1:E:140:ASN:N	2.11	0.48
1:D:5:LEU:HD13	1:D:7:ILE:HD11	1.95	0.48
1:C:17:VAL:HG23	1:C:18:ASP:N	2.28	0.48
1:D:16:ASN:HB2	1:D:18:ASP:OD1	2.12	0.48
1:F:112:GLY:HA2	1:F:122:VAL:HG21	1.94	0.48
1:A:24:ARG:NH2	1:A:28:LYS:NZ	2.61	0.48
1:A:28:LYS:HE2	1:A:86:LEU:HD11	1.94	0.48
1:C:164:GLN:CG	1:C:226:VAL:HG23	2.42	0.48
1:D:146:GLU:HB3	1:D:158:ILE:HD11	1.95	0.48
1:D:209:ARG:O	1:D:213:ILE:HG12	2.13	0.48
1:C:163:THR:O	1:C:167:ARG:HG3	2.13	0.48
1:C:16:ASN:HB3	1:D:53:LEU:CD1	2.43	0.48
1:B:164:GLN:HB2	5:B:2038:HOH:O	2.14	0.48
1:B:16:ASN:ND2	1:B:16:ASN:N	2.62	0.48
1:B:11:PHE:CZ	1:B:19:ASN:HB3	2.49	0.48
1:D:166:LEU:HD12	1:D:166:LEU:N	2.29	0.48
1:E:81:PHE:O	1:E:84:GLN:HG3	2.14	0.48
1:E:114:GLN:O	1:E:117:GLN:HG2	2.13	0.48
1:A:203:ASN:O	1:A:203:ASN:ND2	2.47	0.47
1:F:81:PHE:O	1:F:84:GLN:HG3	2.13	0.47
1:A:141:VAL:HG12	1:A:142:ASP:H	1.79	0.47
1:C:12:PHE:C	1:C:16:ASN:HD21	2.18	0.47
1:E:98:PHE:CD2	1:E:126:VAL:HG22	2.49	0.47
1:C:24:ARG:HA	1:C:83:LEU:HD21	1.95	0.47
1:D:170:LEU:HD21	1:D:184:LEU:HB3	1.95	0.47
1:C:11:PHE:CZ	1:C:19:ASN:HB3	2.49	0.47
1:D:149:PRO:O	1:D:151:ILE:N	2.47	0.47
1:E:183:LEU:HD13	1:E:223:ILE:HD12	1.96	0.47
1:C:205:ARG:HG3	1:C:205:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:ASN:HD21	1:A:206:LYS:HD2	1.79	0.47
1:A:62:ALA:HB2	1:E:128:GLU:HG2	1.95	0.47
1:A:23:LEU:O	1:A:27:ILE:HG13	2.14	0.47
1:B:185:ASP:HB2	1:B:186:PRO:CD	2.36	0.47
1:A:203:ASN:HD21	1:A:206:LYS:CD	2.27	0.47
1:E:25:GLN:CD	1:E:25:GLN:H	2.17	0.47
1:F:141:VAL:CG1	1:F:145:TYR:HE2	2.27	0.47
1:A:204:TYR:O	1:A:204:TYR:HD1	1.98	0.47
1:A:141:VAL:CG1	1:A:145:TYR:HE2	2.27	0.47
1:D:84:GLN:O	1:D:85:ASP:CB	2.62	0.47
1:D:177:GLN:N	1:D:180:THR:HG22	2.30	0.47
1:F:3:ILE:HD11	1:F:136:VAL:HG21	1.95	0.47
1:E:23:LEU:HD12	1:E:26:SER:OG	2.14	0.47
1:A:88:TYR:CE2	1:A:90:HIS:HB3	2.50	0.47
1:D:11:PHE:CE1	1:D:19:ASN:HB2	2.50	0.46
1:A:5:LEU:HD13	1:A:7:ILE:HD11	1.97	0.46
1:F:98:PHE:CD2	1:F:126:VAL:HG22	2.50	0.46
1:D:19:ASN:ND2	5:D:2005:HOH:O	2.47	0.46
1:D:199:VAL:HB	1:D:223:ILE:HB	1.97	0.46
1:A:54:ALA:HB1	1:A:59:ILE:HG13	1.95	0.46
1:A:203:ASN:H	1:A:203:ASN:ND2	2.14	0.46
1:F:98:PHE:CZ	1:F:126:VAL:HG13	2.50	0.46
1:C:183:LEU:O	1:C:184:LEU:HD23	2.15	0.46
1:D:138:ALA:HB1	1:D:204:TYR:HB3	1.97	0.46
1:A:203:ASN:C	1:A:205:ARG:H	2.19	0.46
1:A:203:ASN:HD22	1:A:203:ASN:H	1.63	0.46
1:B:17:VAL:CG2	1:B:18:ASP:N	2.79	0.46
1:E:49:ARG:NH2	1:F:12:PHE:O	2.50	0.45
1:D:213:ILE:HD13	1:D:218:GLU:HB3	1.99	0.45
1:A:146:GLU:OE1	1:A:149:PRO:HA	2.16	0.45
1:A:95:LEU:CD2	1:E:115:PRO:HG2	2.44	0.45
1:B:205:ARG:HG3	1:B:205:ARG:HH11	1.80	0.45
1:F:17:VAL:C	1:F:19:ASN:N	2.69	0.45
1:C:185:ASP:CB	1:C:186:PRO:HD2	2.46	0.45
1:D:99:ILE:HD13	1:F:63:TYR:CE1	2.51	0.45
1:C:145:TYR:CD2	1:C:149:PRO:HD3	2.52	0.45
1:A:10:LYS:HD2	1:A:140:ASN:HB2	1.98	0.45
1:E:66:LEU:HD13	1:E:115:PRO:HG3	1.98	0.45
1:D:100:GLN:HG3	1:E:90:HIS:HB2	1.99	0.45
1:A:157:LEU:HD23	1:A:158:ILE:N	2.32	0.45
1:A:55:ARG:HD2	5:A:2013:HOH:O	2.15	0.45
1:A:82:SER:HA	1:B:59:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:213:ILE:HD13	1:F:218:GLU:HB3	1.99	0.45
1:A:28:LYS:CG	1:A:86:LEU:HD11	2.47	0.45
1:F:5:LEU:HD13	1:F:7:ILE:HD11	1.99	0.45
1:C:206:LYS:NZ	1:C:219:VAL:HB	2.32	0.44
1:B:17:VAL:HG22	5:B:2006:HOH:O	2.17	0.44
1:B:17:VAL:HG23	1:B:18:ASP:N	2.31	0.44
1:F:73:ARG:NH2	1:F:93:GLN:HB3	2.31	0.44
1:B:164:GLN:HG3	1:B:226:VAL:HG21	1.95	0.44
1:D:29:GLU:HB3	1:D:211:ILE:HD11	1.99	0.44
1:F:141:VAL:HG12	1:F:142:ASP:N	2.32	0.44
1:A:1:MET:O	1:A:35:PHE:HA	2.17	0.44
1:E:63:TYR:CD2	1:F:84:GLN:NE2	2.85	0.44
1:C:18:ASP:O	1:C:22:VAL:HG12	2.18	0.44
1:D:19:ASN:ND2	5:D:2004:HOH:O	2.51	0.44
1:E:23:LEU:HD12	1:E:23:LEU:O	2.17	0.44
1:F:16:ASN:HD21	1:F:18:ASP:CG	2.20	0.44
1:A:183:LEU:O	1:A:183:LEU:HD23	2.18	0.44
1:D:3:ILE:CG2	1:D:37:VAL:HG22	2.47	0.44
1:D:208:ASN:OD1	1:D:209:ARG:HG3	2.18	0.44
1:D:210:ILE:O	1:D:213:ILE:HB	2.17	0.44
5:A:2030:HOH:O	1:E:96:GLU:HG3	2.18	0.44
1:B:30:LEU:CD2	1:B:210:ILE:HG21	2.48	0.44
1:F:185:ASP:HA	1:F:186:PRO:HD2	1.88	0.44
1:E:24:ARG:HH11	1:E:24:ARG:CG	2.30	0.44
1:F:4:ILE:HG13	1:F:126:VAL:HG12	1.99	0.43
1:A:139:THR:O	1:A:203:ASN:HA	2.17	0.43
1:D:155:VAL:HG12	1:D:156:LYS:N	2.33	0.43
1:F:178:ALA:C	1:F:180:THR:H	2.22	0.43
1:C:209:ARG:O	1:C:213:ILE:HG12	2.18	0.43
1:E:25:GLN:OE1	1:E:25:GLN:N	2.51	0.43
1:A:49:ARG:NE	5:A:2011:HOH:O	2.51	0.43
1:F:198:ARG:NE	1:F:224:GLU:OE2	2.51	0.43
1:F:142:ASP:CG	1:F:206:LYS:HZ1	2.22	0.43
1:C:16:ASN:HB3	1:D:53:LEU:HD11	2.00	0.43
1:C:161:LEU:N	1:C:161:LEU:HD23	2.33	0.43
1:D:145:TYR:CE1	1:D:157:LEU:HG	2.53	0.43
1:A:204:TYR:O	1:A:204:TYR:CD1	2.70	0.43
1:A:83:LEU:O	1:A:84:GLN:C	2.56	0.43
1:A:25:GLN:HG2	1:A:29:GLU:OE1	2.19	0.43
1:D:182:GLU:O	1:D:183:LEU:HD23	2.18	0.43
1:B:146:GLU:CG	1:B:155:VAL:HG13	2.48	0.43
1:C:40:VAL:HG21	1:C:123:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:13:ASP:C	1:B:16:ASN:HD21	2.21	0.43
1:B:112:GLY:HA3	2:B:227:U5P:C5	2.47	0.43
1:D:95:LEU:HD23	1:F:115:PRO:HG2	2.01	0.43
1:B:167:ARG:NH2	1:B:193:GLU:OE1	2.52	0.43
1:B:161:LEU:HD23	1:B:161:LEU:N	2.33	0.43
1:C:146:GLU:O	1:C:147:LYS:HD2	2.18	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.87	0.42
1:F:140:ASN:HD22	1:F:140:ASN:C	2.23	0.42
1:F:139:THR:HG23	1:F:141:VAL:H	1.84	0.42
1:A:106:LYS:HE3	1:C:103:SER:O	2.18	0.42
1:E:169:ILE:HG21	1:E:184:LEU:HD11	2.01	0.42
1:D:5:LEU:CD1	1:D:7:ILE:HD11	2.48	0.42
1:B:106:LYS:HE3	1:E:103:SER:O	2.19	0.42
1:E:156:LYS:H	1:E:156:LYS:HG2	1.63	0.42
1:F:31:ALA:HA	1:F:35:PHE:O	2.19	0.42
1:B:5:LEU:HD22	1:B:7:ILE:CD1	2.49	0.42
1:D:3:ILE:HG23	1:D:37:VAL:HG22	2.00	0.42
1:C:45:SER:HA	1:C:48:ARG:NH1	2.33	0.42
1:F:204:TYR:O	1:F:207:LEU:HG	2.20	0.42
1:C:217:GLU:O	1:C:218:GLU:HB2	2.19	0.42
1:B:103:SER:O	1:D:106:LYS:HE3	2.20	0.42
1:A:40:VAL:HG21	1:A:123:ALA:HA	2.02	0.42
1:B:139:THR:OG1	1:B:140:ASN:N	2.52	0.42
1:E:22:VAL:C	1:E:25:GLN:NE2	2.72	0.42
1:F:167:ARG:O	1:F:169:ILE:HG22	2.20	0.42
1:A:203:ASN:ND2	1:A:203:ASN:N	2.68	0.42
1:C:65:ASP:O	1:C:69:ILE:HG13	2.20	0.42
1:C:90:HIS:HB2	1:F:100:GLN:HG3	2.02	0.42
1:B:113:PHE:CE2	1:B:122:VAL:HG13	2.54	0.42
1:E:137:VAL:HG11	1:E:182:GLU:HB3	2.01	0.42
1:D:176:VAL:HG23	1:D:184:LEU:HD11	2.00	0.42
1:E:95:LEU:HD21	5:E:2028:HOH:O	2.19	0.42
1:F:5:LEU:HD22	1:F:7:ILE:HD13	2.01	0.42
1:C:66:LEU:HD12	1:C:69:ILE:HD12	2.02	0.42
1:D:24:ARG:O	1:D:28:LYS:HG3	2.20	0.42
1:D:205:ARG:HG3	1:D:205:ARG:NH1	2.35	0.42
1:A:203:ASN:ND2	1:A:206:LYS:HG3	2.35	0.41
1:D:115:PRO:HG2	1:F:95:LEU:CD2	2.50	0.41
1:D:205:ARG:HG3	1:D:205:ARG:HH11	1.83	0.41
1:A:10:LYS:HA	1:A:13:ASP:OD2	2.20	0.41
1:F:140:ASN:HB3	1:F:204:TYR:OH	2.20	0.41
1:C:29:GLU:HG2	1:C:211:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:19:ASN:OD1	1:F:19:ASN:N	2.51	0.41
1:A:157:LEU:C	1:A:157:LEU:HD23	2.40	0.41
1:A:113:PHE:CE2	1:A:122:VAL:HG13	2.55	0.41
1:F:40:VAL:HG22	1:F:110:THR:CG2	2.50	0.41
1:F:90:HIS:ND1	1:F:101:ASP:OD2	2.45	0.41
1:C:95:LEU:HD11	1:C:129:ALA:CB	2.50	0.41
1:D:4:ILE:HG13	1:D:127:ALA:CA	2.51	0.41
1:D:219:VAL:O	1:D:220:SER:HB3	2.20	0.41
1:A:52:LYS:O	1:A:56:GLU:HG3	2.19	0.41
1:C:4:ILE:HG13	1:C:127:ALA:HA	2.03	0.41
1:B:147:LYS:O	1:B:155:VAL:HG11	2.21	0.41
1:C:205:ARG:HG3	1:C:205:ARG:NH1	2.35	0.41
1:E:176:VAL:CG1	1:E:177:GLN:H	2.27	0.41
1:B:24:ARG:HG2	1:B:28:LYS:HE3	2.02	0.41
1:A:128:GLU:HG2	1:E:62:ALA:HB2	2.03	0.41
1:C:50:TYR:OH	1:D:75:ASN:ND2	2.53	0.41
1:E:164:GLN:HA	1:E:167:ARG:HE	1.86	0.41
1:A:5:LEU:CD1	1:A:7:ILE:HD11	2.51	0.41
1:F:6:LYS:HE3	1:F:119:THR:OG1	2.20	0.41
1:B:185:ASP:CB	1:B:186:PRO:CD	2.98	0.41
1:B:206:LYS:CD	1:B:209:ARG:HH21	2.34	0.41
1:B:187:LEU:O	1:B:191:ILE:HG12	2.21	0.41
1:E:187:LEU:O	1:E:191:ILE:HG12	2.20	0.41
1:A:50:TYR:OH	1:B:75:ASN:ND2	2.53	0.41
1:A:141:VAL:CG1	1:A:142:ASP:N	2.82	0.41
1:B:30:LEU:HD21	1:B:210:ILE:HG21	2.02	0.40
1:B:147:LYS:HB3	1:B:152:TYR:CD2	2.55	0.40
1:E:140:ASN:H	1:E:140:ASN:HD22	1.67	0.40
1:C:164:GLN:H	1:C:226:VAL:CG2	2.34	0.40
1:A:194:ARG:CD	1:E:61:GLU:HG2	2.51	0.40
1:F:16:ASN:ND2	1:F:18:ASP:OD1	2.55	0.40
1:B:75:ASN:HD22	1:B:75:ASN:HA	1.73	0.40
1:E:167:ARG:O	1:E:171:GLU:HG3	2.21	0.40
1:B:61:GLU:HG2	1:C:194:ARG:NE	2.37	0.40
1:D:100:GLN:O	1:D:103:SER:CB	2.69	0.40
1:F:83:LEU:O	1:F:84:GLN:C	2.59	0.40
1:E:114:GLN:HA	1:E:115:PRO:HD3	1.93	0.40
1:A:168:LYS:HE3	1:A:168:LYS:CA	2.49	0.40
1:F:98:PHE:CG	1:F:126:VAL:HG22	2.57	0.40
1:F:156:LYS:HG2	1:F:157:LEU:N	2.36	0.40
1:B:88:TYR:CE2	1:B:90:HIS:HB3	2.56	0.40
1:E:40:VAL:HG22	1:E:110:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	201/226 (89%)	189 (94%)	9 (4%)	3 (2%)	15	10
1	B	210/226 (93%)	199 (95%)	10 (5%)	1 (0%)	38	38
1	C	200/226 (88%)	186 (93%)	12 (6%)	2 (1%)	22	18
1	D	224/226 (99%)	210 (94%)	9 (4%)	5 (2%)	10	5
1	E	217/226 (96%)	209 (96%)	7 (3%)	1 (0%)	38	38
1	F	202/226 (89%)	193 (96%)	7 (4%)	2 (1%)	22	18
All	All	1254/1356 (92%)	1186 (95%)	54 (4%)	14 (1%)	21	16

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	149	PRO
1	D	154	ASP
1	A	169	ILE
1	B	16	ASN
1	C	16	ASN
1	D	85	ASP
1	D	150	ARG
1	A	84	GLN
1	A	204	TYR
1	D	29	GLU
1	E	85	ASP
1	F	85	ASP
1	F	84	GLN
1	C	149	PRO

5.3.2 Protein sidechains ⓘ

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	177/192 (92%)	169 (96%)	8 (4%)	38	44
1	B	183/192 (95%)	177 (97%)	6 (3%)	50	60
1	C	176/192 (92%)	169 (96%)	7 (4%)	42	51
1	D	192/192 (100%)	187 (97%)	5 (3%)	59	70
1	E	187/192 (97%)	178 (95%)	9 (5%)	35	41
1	F	176/192 (92%)	165 (94%)	11 (6%)	25	27
All	All	1091/1152 (95%)	1045 (96%)	46 (4%)	40	48

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	16	ASN
1	A	66	LEU
1	A	148	ASP
1	A	168	LYS
1	A	202	MET
1	A	203	ASN
1	B	5	LEU
1	B	66	LEU
1	B	140	ASN
1	B	161	LEU
1	B	198	ARG
1	B	202	MET
1	C	1	MET
1	C	5	LEU
1	C	66	LEU
1	C	140	ASN
1	C	165	ASP
1	C	198	ARG
1	C	202	MET
1	D	5	LEU
1	D	66	LEU

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Mol	Chain	Res	Type
1	D	140	ASN
1	D	161	LEU
1	D	198	ARG
1	E	5	LEU
1	E	24	ARG
1	E	25	GLN
1	E	66	LEU
1	E	140	ASN
1	E	154	ASP
1	E	161	LEU
1	E	185	ASP
1	E	224	GLU
1	F	5	LEU
1	F	19	ASN
1	F	24	ARG
1	F	66	LEU
1	F	85	ASP
1	F	103	SER
1	F	140	ASN
1	F	161	LEU
1	F	185	ASP
1	F	202	MET
1	F	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	33	ASN
1	A	75	ASN
1	A	93	GLN
1	A	114	GLN
1	A	117	GLN
1	A	203	ASN
1	B	16	ASN
1	B	75	ASN
1	B	114	GLN
1	B	117	GLN
1	B	140	ASN
1	C	16	ASN
1	C	33	ASN
1	C	75	ASN

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Mol	Chain	Res	Type
1	C	93	GLN
1	C	114	GLN
1	C	117	GLN
1	C	140	ASN
1	D	16	ASN
1	D	19	ASN
1	D	33	ASN
1	D	75	ASN
1	D	114	GLN
1	D	117	GLN
1	D	140	ASN
1	D	177	GLN
1	E	75	ASN
1	E	114	GLN
1	E	117	GLN
1	E	140	ASN
1	F	33	ASN
1	F	75	ASN
1	F	114	GLN
1	F	117	GLN
1	F	140	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 for Mogul analysis.

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	U5P	A	227	4	22,22,22	5.30	10 (45%)	29,33,33	1.70	5 (17%)
2	U5P	B	227	-	22,22,22	5.42	10 (45%)	29,33,33	1.67	4 (13%)
2	U5P	C	227	-	22,22,22	5.48	11 (50%)	29,33,33	1.65	3 (10%)
2	U5P	D	227	-	22,22,22	5.05	10 (45%)	29,33,33	1.80	5 (17%)
2	U5P	E	227	-	22,22,22	5.25	10 (45%)	29,33,33	1.78	6 (20%)
2	U5P	F	227	-	22,22,22	5.01	10 (45%)	29,33,33	1.74	4 (13%)

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	U5P	A	227	4	-	0/8/26/26	0/2/2/2
2	U5P	B	227	-	-	0/8/26/26	0/2/2/2
2	U5P	C	227	-	-	0/8/26/26	0/2/2/2
2	U5P	D	227	-	-	0/8/26/26	0/2/2/2
2	U5P	E	227	-	-	0/8/26/26	0/2/2/2
2	U5P	F	227	-	-	0/8/26/26	0/2/2/2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	227	U5P	O4-C4	14.80	1.53	1.24
2	B	227	U5P	O4-C4	14.77	1.53	1.24
2	A	227	U5P	O4-C4	14.41	1.52	1.24
2	E	227	U5P	O4-C4	14.33	1.52	1.24
2	F	227	U5P	O4-C4	14.09	1.52	1.24
2	C	227	U5P	C2-N1	13.86	1.53	1.38
2	B	227	U5P	C2-N1	13.75	1.53	1.38
2	A	227	U5P	C2-N1	13.70	1.53	1.38
2	D	227	U5P	O4-C4	13.47	1.50	1.24
2	E	227	U5P	C2-N1	13.41	1.53	1.38
2	D	227	U5P	C2-N1	12.38	1.51	1.38
2	F	227	U5P	C2-N1	11.90	1.51	1.38
2	C	227	U5P	C6-N1	9.61	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	227	U5P	C6-N1	9.51	1.51	1.35
2	B	227	U5P	C6-N1	9.42	1.51	1.35
2	A	227	U5P	C6-N1	9.40	1.51	1.35
2	E	227	U5P	C6-N1	9.18	1.50	1.35
2	F	227	U5P	C6-N1	8.76	1.50	1.35
2	B	227	U5P	O4'-C1'	6.03	1.50	1.41
2	C	227	U5P	O4'-C1'	5.91	1.50	1.41
2	F	227	U5P	C2'-C1'	5.65	1.61	1.53
2	D	227	U5P	C2'-C1'	5.63	1.61	1.53
2	C	227	U5P	C5-C4	5.44	1.54	1.40
2	E	227	U5P	C2'-C1'	5.42	1.61	1.53
2	B	227	U5P	C5-C4	5.39	1.54	1.40
2	A	227	U5P	C5-C4	5.38	1.54	1.40
2	A	227	U5P	C2'-C1'	5.38	1.61	1.53
2	C	227	U5P	C2'-C1'	5.38	1.61	1.53
2	D	227	U5P	C5-C4	5.27	1.54	1.40
2	E	227	U5P	O4'-C1'	5.21	1.49	1.41
2	A	227	U5P	O4'-C1'	5.17	1.49	1.41
2	B	227	U5P	C2'-C1'	5.15	1.60	1.53
2	F	227	U5P	O4'-C1'	5.12	1.49	1.41
2	E	227	U5P	C5-C4	4.88	1.53	1.40
2	D	227	U5P	O4'-C1'	4.85	1.48	1.41
2	F	227	U5P	C5-C4	4.52	1.52	1.40
2	C	227	U5P	C4-N3	4.33	1.44	1.37
2	F	227	U5P	C4-N3	4.11	1.44	1.37
2	B	227	U5P	C4-N3	3.96	1.43	1.37
2	E	227	U5P	C4-N3	3.92	1.43	1.37
2	D	227	U5P	C4-N3	3.75	1.43	1.37
2	A	227	U5P	C4-N3	3.44	1.43	1.37
2	D	227	U5P	O4'-C4'	-3.35	1.37	1.45
2	E	227	U5P	O4'-C4'	-3.25	1.37	1.45
2	B	227	U5P	O4'-C4'	-3.11	1.37	1.45
2	A	227	U5P	O4'-C4'	-3.09	1.37	1.45
2	C	227	U5P	O4'-C4'	-2.99	1.38	1.45
2	F	227	U5P	O4'-C4'	-2.97	1.38	1.45
2	C	227	U5P	C2-N3	2.92	1.43	1.37
2	C	227	U5P	C1'-N1	2.86	1.57	1.48
2	E	227	U5P	C1'-N1	2.84	1.57	1.48
2	B	227	U5P	C2-N3	2.80	1.42	1.37
2	F	227	U5P	C1'-N1	2.75	1.57	1.48
2	E	227	U5P	C2-N3	2.72	1.42	1.37
2	A	227	U5P	C1'-N1	2.70	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	227	U5P	C1'-N1	2.66	1.57	1.48
2	D	227	U5P	C1'-N1	2.42	1.56	1.48
2	F	227	U5P	C2-N3	2.40	1.42	1.37
2	A	227	U5P	C2-N3	2.17	1.41	1.37
2	C	227	U5P	C6-C5	2.13	1.39	1.36
2	D	227	U5P	C2-N3	2.04	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	227	U5P	O2'-C2'-C3'	5.47	129.63	111.83
2	C	227	U5P	O2'-C2'-C3'	5.43	129.51	111.83
2	A	227	U5P	O2'-C2'-C3'	5.41	129.44	111.83
2	D	227	U5P	O2'-C2'-C3'	5.34	129.22	111.83
2	F	227	U5P	O2'-C2'-C3'	5.28	129.02	111.83
2	E	227	U5P	O2'-C2'-C3'	5.24	128.89	111.83
2	E	227	U5P	C5-C6-N1	3.40	125.06	121.21
2	F	227	U5P	C5-C6-N1	3.35	125.01	121.21
2	C	227	U5P	C5-C6-N1	3.16	124.79	121.21
2	B	227	U5P	C5-C6-N1	2.98	124.58	121.21
2	D	227	U5P	C5-C6-N1	2.97	124.57	121.21
2	A	227	U5P	C5-C6-N1	2.97	124.57	121.21
2	E	227	U5P	O4'-C1'-C2'	-2.79	102.50	106.77
2	F	227	U5P	O4'-C1'-C2'	-2.71	102.61	106.77
2	D	227	U5P	O4'-C1'-C2'	-2.69	102.64	106.77
2	D	227	U5P	C3'-C2'-C1'	-2.53	96.94	100.91
2	A	227	U5P	O4'-C1'-C2'	-2.36	103.15	106.77
2	E	227	U5P	C4'-O4'-C1'	2.31	112.26	109.75
2	B	227	U5P	O4'-C1'-C2'	-2.28	103.28	106.77
2	B	227	U5P	C3'-C2'-C1'	-2.27	97.35	100.91
2	E	227	U5P	N3-C2-N1	-2.24	114.11	115.97
2	A	227	U5P	C4'-O4'-C1'	2.22	112.16	109.75
2	F	227	U5P	C3'-C2'-C1'	-2.20	97.46	100.91
2	E	227	U5P	C3'-C2'-C1'	-2.10	97.63	100.91
2	C	227	U5P	O4'-C1'-C2'	-2.04	103.64	106.77
2	D	227	U5P	O4'-C4'-C5'	-2.00	102.20	109.36
2	A	227	U5P	C3'-C2'-C1'	-2.00	97.77	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	207/226 (91%)	0.58	27 (13%) 4 4	14, 30, 70, 85	0
1	B	214/226 (94%)	0.32	15 (7%) 16 16	17, 30, 55, 67	0
1	C	206/226 (91%)	0.73	29 (14%) 3 3	17, 31, 67, 88	0
1	D	226/226 (100%)	0.58	25 (11%) 6 5	15, 32, 65, 73	0
1	E	221/226 (97%)	0.53	25 (11%) 6 5	14, 28, 66, 72	0
1	F	208/226 (92%)	0.44	19 (9%) 9 9	14, 27, 58, 76	0
All	All	1282/1356 (94%)	0.53	140 (10%) 6 6	14, 30, 64, 88	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	10.8
1	A	170	LEU	7.1
1	C	149	PRO	7.0
1	C	164	GLN	6.9
1	C	150	ARG	6.5
1	C	152	TYR	6.4
1	E	173	SER	6.3
1	B	15	ASP	6.0
1	A	148	ASP	5.7
1	C	151	ILE	5.6
1	A	150	ARG	5.5
1	F	181	TYR	5.5
1	D	152	TYR	5.4
1	A	226	VAL	5.2
1	C	148	ASP	5.2
1	C	1	MET	4.9
1	C	15	ASP	4.9
1	D	226	VAL	4.8
1	C	147	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	164	GLN	4.8
1	D	85	ASP	4.7
1	E	174	GLN	4.7
1	D	15	ASP	4.6
1	C	146	GLU	4.6
1	C	166	LEU	4.5
1	B	14	GLU	4.5
1	E	172	GLY	4.4
1	D	170	LEU	4.4
1	D	150	ARG	4.3
1	C	225	PRO	4.3
1	F	217	GLU	4.3
1	E	154	ASP	4.2
1	B	150	ARG	4.2
1	A	209	ARG	4.1
1	A	147	LYS	4.1
1	D	32	ASP	4.1
1	E	15	ASP	4.1
1	A	218	GLU	4.0
1	E	32	ASP	4.0
1	E	153	ALA	3.9
1	D	151	ILE	3.9
1	E	175	SER	3.9
1	B	32	ASP	3.8
1	A	168	LYS	3.8
1	A	203	ASN	3.8
1	A	15	ASP	3.7
1	F	15	ASP	3.7
1	E	176	VAL	3.7
1	A	153	ALA	3.6
1	A	169	ILE	3.6
1	F	226	VAL	3.6
1	A	167	ARG	3.6
1	F	179	GLY	3.6
1	A	149	PRO	3.5
1	C	85	ASP	3.5
1	C	14	GLU	3.5
1	D	181	TYR	3.4
1	A	164	GLN	3.4
1	F	32	ASP	3.3
1	E	156	LYS	3.3
1	A	146	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	171	GLU	3.3
1	F	1	MET	3.3
1	F	169	ILE	3.3
1	B	168	LYS	3.2
1	E	168	LYS	3.1
1	A	152	TYR	3.1
1	E	147	LYS	3.1
1	B	154	ASP	3.0
1	C	136	VAL	3.0
1	F	33	ASN	3.0
1	F	184	LEU	3.0
1	B	1	MET	2.9
1	C	217	GLU	2.9
1	B	226	VAL	2.9
1	D	154	ASP	2.9
1	A	210	ILE	2.9
1	D	21	ILE	2.8
1	E	85	ASP	2.8
1	D	153	ALA	2.8
1	A	33	ASN	2.8
1	A	85	ASP	2.8
1	C	158	ILE	2.8
1	E	22	VAL	2.8
1	B	85	ASP	2.7
1	D	172	GLY	2.7
1	A	140	ASN	2.7
1	E	181	TYR	2.7
1	D	149	PRO	2.7
1	A	155	VAL	2.6
1	C	163	THR	2.6
1	D	31	ALA	2.6
1	F	178	ALA	2.6
1	D	33	ASN	2.6
1	E	34	GLY	2.6
1	E	150	ARG	2.6
1	C	32	ASP	2.5
1	F	209	ARG	2.5
1	A	25	GLN	2.5
1	E	29	GLU	2.5
1	B	169	ILE	2.5
1	A	141	VAL	2.5
1	F	199	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	171	GLU	2.5
1	B	182	GLU	2.5
1	E	223	ILE	2.5
1	D	173	SER	2.4
1	D	217	GLU	2.4
1	C	144	VAL	2.4
1	C	140	ASN	2.4
1	B	217	GLU	2.4
1	D	167	ARG	2.4
1	C	13	ASP	2.4
1	F	18	ASP	2.4
1	F	34	GLY	2.3
1	F	218	GLU	2.3
1	F	30	LEU	2.3
1	F	222	ILE	2.3
1	C	165	ASP	2.3
1	D	178	ALA	2.3
1	D	20	LEU	2.2
1	C	186	PRO	2.2
1	E	217	GLU	2.2
1	B	165	ASP	2.2
1	C	185	ASP	2.2
1	C	218	GLU	2.1
1	F	168	LYS	2.1
1	D	22	VAL	2.1
1	E	199	VAL	2.1
1	E	226	VAL	2.1
1	A	32	ASP	2.1
1	E	155	VAL	2.1
1	B	156	LYS	2.1
1	D	155	VAL	2.0
1	E	136	VAL	2.0
1	D	5	LEU	2.0
1	A	205	ARG	2.0
1	A	219	VAL	2.0
1	C	133	LYS	2.0
1	C	29	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	U5P	C	227	21/21	0.26	4.18	48,59,60,61	0
4	MG	A	231	1/1	0.13	2.55	33,33,33,33	0
2	U5P	B	227	21/21	0.17	2.31	30,43,47,49	0
2	U5P	A	227	21/21	0.14	1.02	26,32,37,39	0
2	U5P	E	227	21/21	0.11	-0.15	22,26,29,30	0
2	U5P	F	227	21/21	0.11	-0.25	18,23,28,32	0
2	U5P	D	227	21/21	0.10	-1.06	13,23,28,29	0
3	CD	B	234	1/1	0.06	-1.38	61,61,61,61	1
3	CD	C	231	1/1	0.05	-1.63	56,56,56,56	1
3	CD	A	230	1/1	0.04	-1.68	102,102,102,102	0
3	CD	B	232	1/1	0.07	-1.78	131,131,131,131	0
3	CD	B	231	1/1	0.04	-2.44	80,80,80,80	0
3	CD	A	229	1/1	0.05	-2.85	43,43,43,43	0
3	CD	B	230	1/1	0.07	-3.15	78,78,78,78	0
3	CD	F	229	1/1	0.05	-3.15	52,52,52,52	0
3	CD	A	228	1/1	0.07	-3.21	27,27,27,27	0
3	CD	C	228	1/1	0.04	-3.50	49,49,49,49	0
3	CD	B	228	1/1	0.06	-4.17	23,23,23,23	0
3	CD	E	228	1/1	0.03	-4.84	42,42,42,42	0
3	CD	B	233	1/1	0.04	-5.31	45,45,45,45	0
3	CD	E	229	1/1	0.07	-5.69	47,47,47,47	0
3	CD	B	229	1/1	0.03	-7.25	46,46,46,46	0
3	CD	D	228	1/1	0.02	-7.92	41,41,41,41	0
3	CD	C	229	1/1	0.03	-8.90	78,78,78,78	0
3	CD	F	228	1/1	0.04	-10.78	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.