



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:17 PM GMT

PDB ID : 1JLS
Title : STRUCTURE OF THE URACIL PHOSPHORIBOSYLTRANSFERASE
URACIL/CPR 2 MUTANT C128V
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Brennan, R.G.
Deposited on : 2001-07-16
Resolution : 2.50 Å(reported)

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

The following versions of software and data (see [references ⓘ](#)) 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

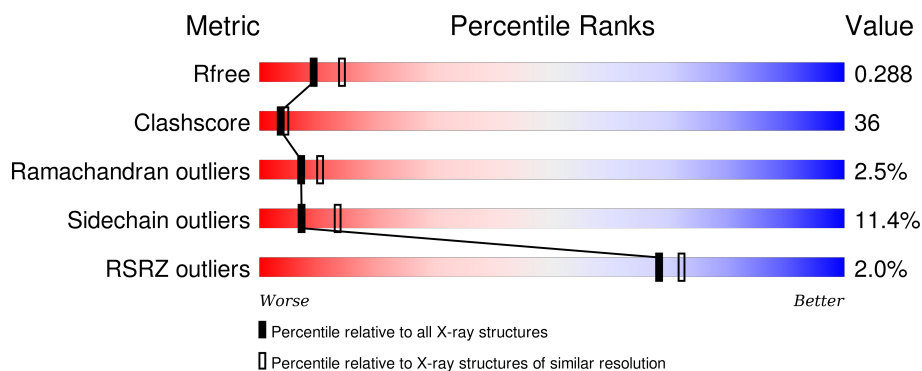
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	243	
1	B	243	
1	C	243	
1	D	243	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1599	-	-	X	-
2	PO4	A	3599	-	-	-	X
2	PO4	B	3699	-	-	X	-
2	PO4	C	2599	-	-	X	-
2	PO4	D	3799	-	-	X	-
4	URA	B	300	-	-	X	X
5	PRP	B	301	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7286 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.

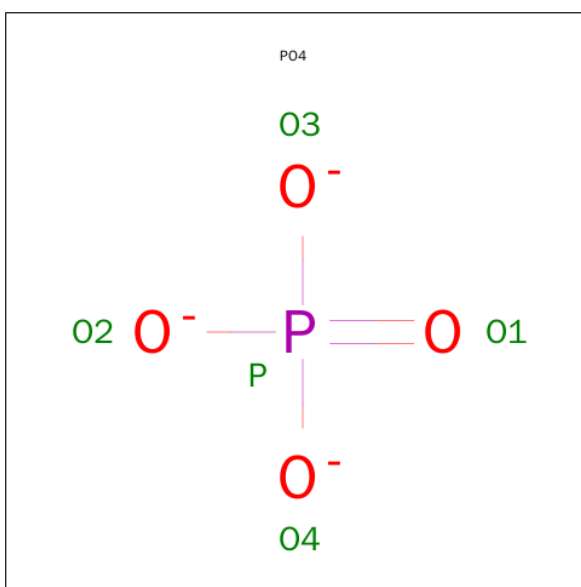
- Molecule 1 is a protein called Uracil phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	224	Total	C	N	O	S	0	0	0
			1787	1146	305	323	13			
1	A	219	Total	C	N	O	S	0	0	0
			1751	1125	300	314	12			
1	D	219	Total	C	N	O	S	0	0	0
			1751	1125	300	314	12			
1	C	223	Total	C	N	O	S	0	0	0
			1779	1141	304	322	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	84	GLN	GLU	CONFLICT	UNP Q26998
B	128	VAL	CYS	ENGINEERED	UNP Q26998
B	157	GLU	ASP	CONFLICT	UNP Q26998
A	84	GLN	GLU	CONFLICT	UNP Q26998
A	128	VAL	CYS	ENGINEERED	UNP Q26998
A	157	GLU	ASP	CONFLICT	UNP Q26998
D	84	GLN	GLU	CONFLICT	UNP Q26998
D	128	VAL	CYS	ENGINEERED	UNP Q26998
D	157	GLU	ASP	CONFLICT	UNP Q26998
C	84	GLN	GLU	CONFLICT	UNP Q26998
C	128	VAL	CYS	ENGINEERED	UNP Q26998
C	157	GLU	ASP	CONFLICT	UNP Q26998

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

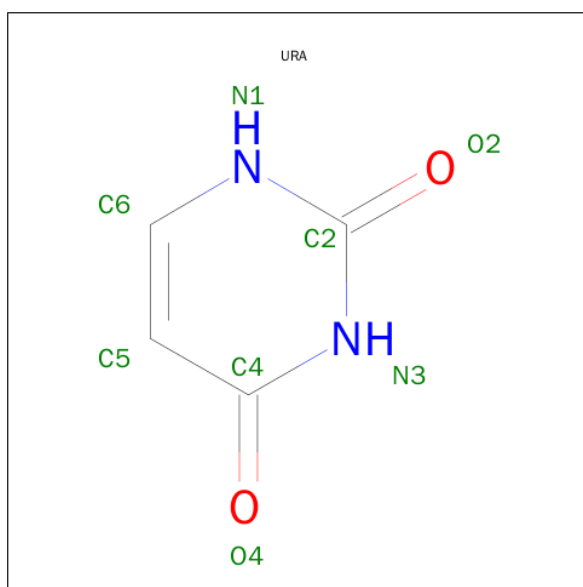


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

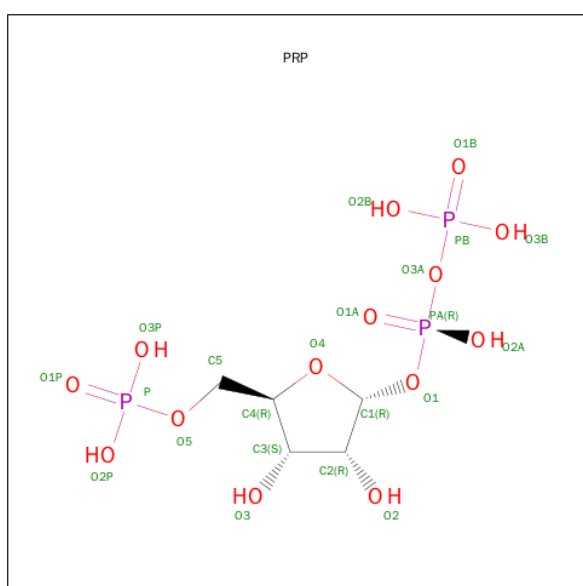
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is URACIL (three-letter code: URA) (formula: C₄H₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	2	2		
4	A	1	Total	C	N	O	0	0
			8	4	2	2		
4	D	1	Total	C	N	O	0	0
			8	4	2	2		
4	C	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 5 is ALPHA-PHOSPHORIBOSYLPYROPHOSPHORIC ACID (three-letter code: PRP) (formula: $C_5H_{13}O_{14}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			22	5	14	3		

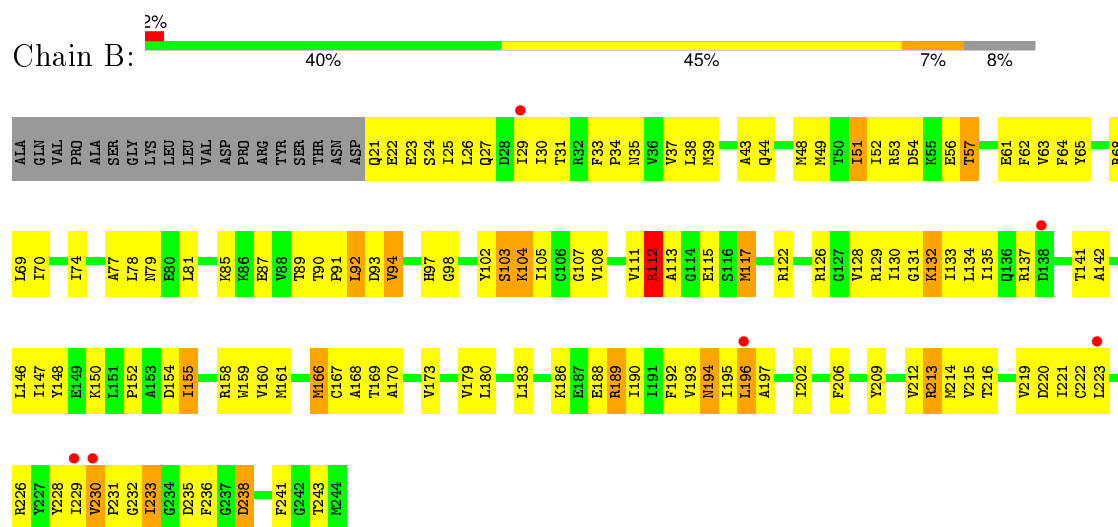
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	35	Total	O	0	0
			35	35		
6	B	24	Total	O	0	0
			24	24		
6	C	21	Total	O	0	0
			21	21		
6	D	38	Total	O	0	0
			38	38		

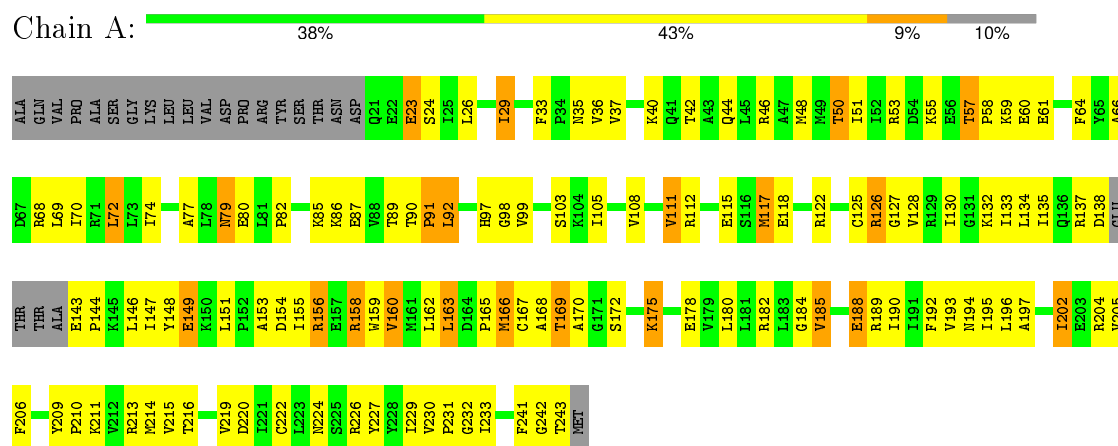
3 Residue-property plots

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: Uracil phosphoribosyltransferase

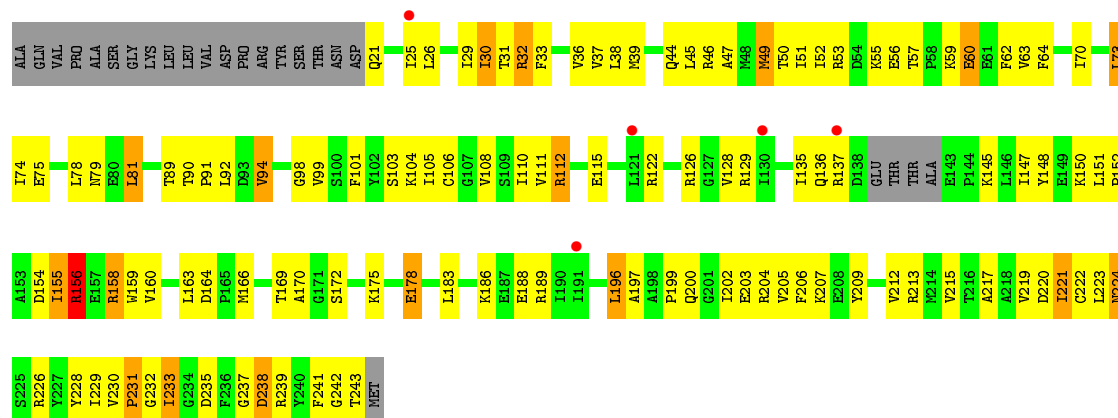


- Molecule 1: Uracil phosphoribosyltransferase

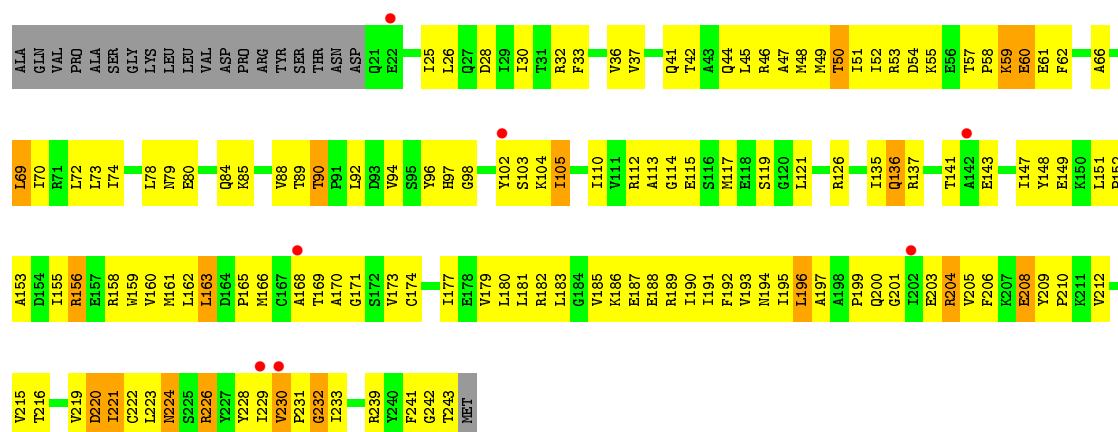


- Molecule 1: Uracil phosphoribosyltransferase





• Molecule 1: Uracil phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.40Å 111.40Å 71.90Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	60.03 – 2.50 60.02 – 2.32	Depositor EDS
% Data completeness (in resolution range)	84.6 (60.03-2.50) 77.5 (60.02-2.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.32Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.288 0.231 , 0.288	Depositor DCC
R_{free} test set	3240 reflections (11.00%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.1	EDS
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37359 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7286	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, PRP, URA

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	0.46	0/1779	0.71	0/2398
1	B	0.44	0/1816	0.74	2/2450 (0.1%)
1	C	0.44	0/1808	0.73	1/2440 (0.0%)
1	D	0.45	0/1779	0.71	0/2398
All	All	0.45	0/7182	0.72	3/9686 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	VAL	C-N-CD	7.46	144.08	128.40
1	C	230	VAL	C-N-CD	6.46	141.96	128.40
1	B	230	VAL	C-N-CA	-5.12	100.50	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1751	0	1822	130	0
1	B	1787	0	1857	151	0
1	C	1779	0	1848	152	0
1	D	1751	0	1822	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	4	0
2	B	5	0	0	4	0
2	C	10	0	0	3	0
2	D	15	0	0	4	0
3	B	1	0	0	0	0
4	A	8	0	3	0	0
4	B	8	0	3	6	0
4	C	8	0	3	1	0
4	D	8	0	3	0	0
5	B	22	0	8	1	0
6	A	35	0	0	3	0
6	B	24	0	0	4	0
6	C	21	0	0	8	0
6	D	38	0	0	4	0
All	All	7286	0	7369	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (521) 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:230:VAL:HG23	1:C:231:PRO:HD3	1.22	1.17
1:B:113:ALA:HB3	6:B:830:HOH:O	1.54	1.06
1:B:230:VAL:HG23	1:B:231:PRO:HD3	1.07	1.05
1:B:230:VAL:HG23	1:B:231:PRO:CD	1.89	1.02
1:D:51:ILE:HG13	1:D:57:THR:HG21	1.47	0.95
1:B:230:VAL:CG2	1:B:231:PRO:HD3	1.95	0.95
1:C:156:ARG:H	1:C:156:ARG:HD2	1.29	0.93
1:A:90:THR:HG22	1:A:92:LEU:H	1.31	0.92
1:C:169:THR:HG23	1:C:171:GLY:H	1.32	0.90
1:B:90:THR:HG22	1:B:92:LEU:H	1.37	0.89
1:C:230:VAL:HG23	1:C:231:PRO:CD	2.02	0.89
1:B:79:ASN:HD21	1:C:44:GLN:H	1.21	0.89
1:C:105:ILE:HG22	1:C:159:TRP:HB2	1.53	0.89
1:D:159:TRP:HA	1:D:189:ARG:HG2	1.55	0.88
1:D:238:ASP:HB2	1:D:243:THR:HA	1.55	0.87
1:A:42:THR:HB	1:D:79:ASN:HD21	1.42	0.84
1:B:54:ASP:HB3	1:B:57:THR:HG22	1.58	0.84
1:A:85:LYS:HD3	1:A:86:LYS:H	1.43	0.83
1:A:51:ILE:O	1:A:57:THR:HG21	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG21	1:D:231:PRO:O	1.78	0.83
1:B:105:ILE:HG22	1:B:159:TRP:HB2	1.60	0.82
1:D:112:ARG:H	1:D:115:GLU:HG3	1.44	0.81
1:C:163:LEU:HD12	1:C:193:VAL:HB	1.62	0.81
1:C:137:ARG:NH2	1:C:169:THR:HG21	1.96	0.80
1:C:110:ILE:HD11	1:C:162:LEU:HD11	1.62	0.80
1:A:29:ILE:HD11	1:A:219:VAL:HG11	1.62	0.79
1:D:155:ILE:HG23	1:D:156:ARG:H	1.48	0.79
1:A:44:GLN:HE21	1:A:68:ARG:HH22	1.31	0.79
1:C:90:THR:HG23	1:C:92:LEU:H	1.49	0.78
1:B:167:CYS:HB3	1:B:197:ALA:HB1	1.65	0.78
1:B:112:ARG:H	1:B:115:GLU:HG3	1.51	0.76
1:A:231:PRO:O	1:D:90:THR:HG21	1.86	0.76
1:C:73:LEU:HD22	1:C:195:ILE:HD13	1.69	0.75
1:A:85:LYS:HD3	1:A:86:LYS:N	2.01	0.75
1:A:33:PHE:O	1:A:36:VAL:HG12	1.87	0.75
1:A:156:ARG:HD2	1:A:156:ARG:H	1.51	0.75
1:D:155:ILE:HG23	1:D:156:ARG:N	2.00	0.75
1:B:167:CYS:HB3	1:B:197:ALA:CB	2.17	0.75
1:D:104:LYS:HG2	2:D:3799:PO4:O1	1.87	0.74
1:A:48:MET:HE3	1:A:68:ARG:HG2	1.70	0.74
1:A:40:LYS:HE3	1:A:42:THR:HG22	1.69	0.73
1:A:180:LEU:O	1:A:185:VAL:HG12	1.87	0.73
1:C:37:VAL:HB	1:C:215:VAL:HG22	1.69	0.73
1:B:194:ASN:O	1:B:216:THR:HA	1.89	0.73
1:A:33:PHE:CD2	1:A:202:ILE:HD11	2.23	0.73
1:D:60:GLU:H	1:D:60:GLU:CD	1.91	0.73
1:D:221:ILE:HD12	1:D:221:ILE:O	1.90	0.72
1:C:230:VAL:O	1:C:231:PRO:C	2.22	0.71
1:B:159:TRP:CD2	1:B:189:ARG:HG3	2.24	0.71
1:B:146:LEU:O	1:B:147:ILE:HD12	1.90	0.71
1:B:79:ASN:ND2	1:C:44:GLN:H	1.88	0.71
1:C:49:MET:O	1:C:53:ARG:HG3	1.90	0.71
1:D:242:GLY:O	6:D:704:HOH:O	2.08	0.71
1:C:46:ARG:O	1:C:50:THR:HG22	1.91	0.70
1:A:226:ARG:NE	1:A:226:ARG:HA	2.07	0.70
1:D:104:LYS:HG2	2:D:3799:PO4:P	2.32	0.70
1:C:25:ILE:HG12	1:C:221:ILE:HG12	1.72	0.70
1:A:42:THR:HB	1:D:79:ASN:ND2	2.06	0.70
1:D:224:ASN:ND2	1:D:228:TYR:H	1.91	0.69
1:A:23:GLU:HG3	1:A:24:SER:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:VAL:O	1:B:112:ARG:HB2	1.92	0.68
1:B:231:PRO:O	1:C:90:THR:HG21	1.94	0.68
1:D:222:CYS:O	1:D:230:VAL:HG22	1.92	0.68
1:B:233:ILE:O	1:B:233:ILE:HD13	1.93	0.67
1:D:238:ASP:HB2	1:D:243:THR:CA	2.25	0.67
1:B:27:GLN:O	1:B:30:ILE:HG22	1.93	0.67
1:A:66:ALA:O	1:A:70:ILE:HG12	1.95	0.66
1:D:230:VAL:HA	1:D:231:PRO:C	2.16	0.66
1:B:21:GLN:OE1	1:B:24:SER:HB2	1.95	0.66
1:C:85:LYS:HD2	1:C:98:GLY:O	1.95	0.66
1:A:153:ALA:O	1:A:156:ARG:NH1	2.29	0.66
1:D:90:THR:HG23	1:D:92:LEU:H	1.61	0.66
1:A:194:ASN:O	1:A:216:THR:HA	1.96	0.65
1:D:106:CYS:SG	1:D:160:VAL:HG22	2.37	0.65
1:B:122:ARG:HG2	1:B:128:VAL:HG12	1.77	0.65
1:B:159:TRP:CE2	1:B:189:ARG:HG3	2.30	0.65
1:A:156:ARG:HD2	1:A:156:ARG:N	2.12	0.64
1:C:196:LEU:HD23	1:C:197:ALA:H	1.61	0.64
1:B:54:ASP:C	1:B:56:GLU:H	2.01	0.64
1:C:26:LEU:O	1:C:30:ILE:HG12	1.97	0.64
1:B:51:ILE:O	1:B:57:THR:HG21	1.98	0.64
1:B:51:ILE:HG12	1:B:65:TYR:CD2	2.33	0.64
1:A:44:GLN:NE2	6:A:826:HOH:O	2.30	0.64
1:D:112:ARG:HD3	1:C:148:TYR:OH	1.98	0.63
1:A:48:MET:CE	1:A:68:ARG:HG2	2.26	0.63
1:D:49:MET:HA	1:D:52:ILE:HG22	1.79	0.63
1:C:161:MET:CE	1:C:191:ILE:HD12	2.28	0.63
1:B:104:LYS:CG	1:B:158:ARG:HH21	2.12	0.63
1:D:199:PRO:HD3	1:D:220:ASP:O	1.98	0.63
1:C:88:VAL:HG23	1:C:96:TYR:HB3	1.80	0.63
1:A:180:LEU:HB3	1:A:185:VAL:HG11	1.81	0.63
1:A:122:ARG:HG2	1:A:128:VAL:HG12	1.80	0.62
1:B:241:PHE:HA	1:A:122:ARG:HH22	1.63	0.62
1:C:54:ASP:O	1:C:57:THR:HG22	1.99	0.62
1:A:99:VAL:HG13	1:D:46:ARG:HG2	1.82	0.62
1:A:53:ARG:HG2	1:A:233:ILE:HG12	1.81	0.62
1:D:52:ILE:HG13	1:D:62:PHE:CE1	2.35	0.62
1:A:163:LEU:HD12	1:A:193:VAL:HB	1.82	0.62
1:C:186:LYS:HA	1:C:186:LYS:HE2	1.82	0.62
1:A:122:ARG:HD2	6:A:779:HOH:O	2.00	0.62
1:A:50:THR:HG21	1:D:99:VAL:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ALA:HB2	1:B:215:VAL:HG11	1.82	0.61
1:A:137:ARG:HD3	1:A:144:PRO:HG3	1.82	0.61
1:B:202:ILE:HG13	1:B:214:MET:CE	2.30	0.61
1:D:224:ASN:HD21	1:D:228:TYR:H	1.48	0.61
1:C:48:MET:HE2	1:C:69:LEU:HB2	1.81	0.61
1:B:235:ASP:OD2	1:B:238:ASP:HB2	2.01	0.61
1:D:200:GLN:HE21	1:D:223:LEU:HD13	1.65	0.61
1:C:156:ARG:HD2	1:C:156:ARG:N	2.11	0.60
1:D:156:ARG:HB2	1:D:156:ARG:CZ	2.31	0.60
1:A:105:ILE:HG22	1:A:159:TRP:HB2	1.83	0.60
1:B:25:ILE:HD12	1:B:221:ILE:HG22	1.82	0.60
1:B:70:ILE:HD11	1:B:195:ILE:HD11	1.82	0.60
1:A:87:GLU:OE1	1:A:97:HIS:HD2	1.85	0.60
1:B:104:LYS:HD3	2:B:3699:PO4:O2	2.02	0.60
1:C:169:THR:HG23	1:C:171:GLY:N	2.12	0.59
1:C:161:MET:HE1	1:C:191:ILE:HD12	1.84	0.59
1:B:69:LEU:HD21	1:B:195:ILE:HG23	1.82	0.59
1:B:43:ALA:H	1:C:79:ASN:HD21	1.51	0.59
1:B:166:MET:HE2	4:B:300:URA:H3	1.66	0.59
1:C:169:THR:HG22	2:C:2599:PO4:O4	2.02	0.59
1:D:135:ILE:HD13	1:D:175:LYS:HB3	1.84	0.59
1:D:29:ILE:HD12	1:D:30:ILE:N	2.18	0.59
1:C:112:ARG:HH12	1:C:243:THR:HG21	1.68	0.59
1:B:196:LEU:HD11	1:B:232:GLY:HA2	1.85	0.59
1:C:115:GLU:N	6:C:825:HOH:O	2.34	0.58
1:A:46:ARG:O	1:A:50:THR:HG23	2.02	0.58
1:D:81:LEU:O	1:D:101:PHE:HE2	1.86	0.58
1:A:89:THR:O	1:D:55:LYS:HG2	2.03	0.58
1:D:152:PRO:HA	1:C:243:THR:HA	1.86	0.58
1:D:203:GLU:O	1:D:207:LYS:HE3	2.03	0.58
1:D:178:GLU:HB3	1:D:209:TYR:OH	2.03	0.58
1:B:196:LEU:HD22	1:B:197:ALA:N	2.18	0.58
1:B:111:VAL:HG21	1:B:134:LEU:HB2	1.86	0.58
1:B:92:LEU:O	1:B:94:VAL:HG12	2.03	0.58
1:D:196:LEU:HD12	1:D:233:ILE:HG23	1.84	0.58
1:B:90:THR:HG23	1:B:91:PRO:HD2	1.84	0.58
1:B:186:LYS:HG2	6:B:839:HOH:O	2.02	0.58
1:A:40:LYS:HE3	1:A:42:THR:CG2	2.33	0.58
1:C:90:THR:CG2	1:C:92:LEU:H	2.16	0.58
1:B:85:LYS:HD2	1:B:98:GLY:O	2.03	0.58
1:C:51:ILE:O	1:C:57:THR:HG21	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HD2	1:B:142:ALA:O	2.04	0.57
1:D:33:PHE:O	1:D:36:VAL:HG22	2.04	0.57
1:D:215:VAL:HG13	1:D:215:VAL:O	2.03	0.57
1:B:166:MET:HG2	4:B:300:URA:H3	1.70	0.57
1:D:186:LYS:HB3	1:D:188:GLU:OE2	2.04	0.57
1:D:73:LEU:HD21	1:D:217:ALA:HB2	1.87	0.57
1:D:155:ILE:CG2	1:D:156:ARG:H	2.16	0.57
1:C:226:ARG:HB3	1:C:228:TYR:HD1	1.70	0.57
1:C:208:GLU:O	1:C:210:PRO:HD3	2.05	0.57
1:A:156:ARG:CD	1:A:156:ARG:H	2.18	0.57
1:B:169:THR:OG1	5:B:301:PRP:O3P	2.17	0.57
1:B:235:ASP:HB3	1:B:238:ASP:HB2	1.85	0.57
1:C:186:LYS:HB2	1:C:189:ARG:HB2	1.86	0.56
1:B:43:ALA:N	1:C:79:ASN:HD21	2.02	0.56
1:B:129:ARG:HG2	1:A:242:GLY:HA3	1.85	0.56
1:B:112:ARG:N	1:B:115:GLU:HG3	2.19	0.56
1:B:166:MET:CE	4:B:300:URA:H3	2.17	0.56
1:C:233:ILE:HG22	1:C:233:ILE:O	2.03	0.56
1:C:73:LEU:CD2	1:C:195:ILE:HD13	2.35	0.56
1:D:188:GLU:H	1:D:188:GLU:CD	2.08	0.56
1:C:180:LEU:HB3	1:C:185:VAL:HG21	1.88	0.56
1:C:169:THR:HG22	2:C:2599:PO4:P	2.46	0.56
1:B:111:VAL:HB	1:B:134:LEU:HD13	1.87	0.56
1:A:80:GLU:HG3	1:A:213:ARG:HG2	1.86	0.56
1:C:33:PHE:O	1:C:36:VAL:HG12	2.05	0.56
1:B:243:THR:HG21	6:B:770:HOH:O	2.06	0.56
1:C:187:GLU:CD	1:C:209:TYR:HB3	2.26	0.55
1:B:62:PHE:CZ	1:B:233:ILE:HD11	2.41	0.55
1:B:202:ILE:HG13	1:B:214:MET:HE1	1.88	0.55
1:C:59:LYS:O	1:C:61:GLU:N	2.39	0.55
1:B:134:LEU:HD12	6:B:706:HOH:O	2.05	0.55
1:C:177:ILE:HA	1:C:180:LEU:HD12	1.87	0.55
1:A:112:ARG:H	1:A:115:GLU:HG3	1.71	0.55
1:B:159:TRP:CZ3	1:B:189:ARG:HA	2.42	0.55
1:B:159:TRP:CE3	1:B:189:ARG:HA	2.42	0.55
1:D:112:ARG:N	1:D:115:GLU:HG3	2.17	0.55
1:D:148:TYR:OH	1:C:112:ARG:HD3	2.05	0.55
1:D:155:ILE:CG2	1:D:156:ARG:N	2.70	0.55
1:B:148:TYR:OH	1:A:112:ARG:HD3	2.06	0.55
1:D:151:LEU:HD12	1:D:183:LEU:CD1	2.37	0.55
1:B:27:GLN:O	1:B:31:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:MET:HG2	4:B:300:URA:N3	2.21	0.55
1:C:102:TYR:O	1:C:103:SER:HB2	2.06	0.55
1:C:222:CYS:O	1:C:230:VAL:HG22	2.07	0.55
1:C:119:SER:N	6:C:820:HOH:O	2.38	0.55
1:C:85:LYS:HE3	1:C:97:HIS:HB3	1.89	0.54
1:C:166:MET:HG3	4:C:600:URA:C2	2.42	0.54
1:B:74:ILE:O	1:B:78:LEU:HG	2.07	0.54
1:C:151:LEU:HB3	1:C:155:ILE:HD12	1.88	0.54
1:B:179:VAL:O	1:B:183:LEU:HG	2.06	0.54
1:A:74:ILE:O	1:A:77:ALA:HB3	2.07	0.54
1:B:104:LYS:HG3	1:B:158:ARG:HH21	1.71	0.54
1:C:47:ALA:O	1:C:50:THR:HG23	2.07	0.54
1:A:72:LEU:HD21	1:D:75:GLU:HG3	1.87	0.54
1:D:203:GLU:O	1:D:207:LYS:HB2	2.07	0.54
1:B:154:ASP:HB3	1:B:158:ARG:HH11	1.72	0.54
1:A:26:LEU:HD12	1:A:219:VAL:HG13	1.90	0.54
1:B:196:LEU:HD13	1:B:229:ILE:HD13	1.90	0.54
1:D:30:ILE:HG22	1:D:31:THR:HG23	1.89	0.54
1:D:151:LEU:HD12	1:D:183:LEU:HD12	1.89	0.54
1:B:30:ILE:HG22	1:B:31:THR:HG23	1.89	0.53
1:B:241:PHE:HA	1:A:122:ARG:NH2	2.22	0.53
1:A:137:ARG:HH12	1:A:172:SER:HB3	1.73	0.53
1:B:230:VAL:O	1:B:231:PRO:C	2.42	0.53
1:B:70:ILE:HG21	1:B:117:MET:HA	1.90	0.53
1:A:162:LEU:HB3	1:A:192:PHE:HA	1.90	0.53
1:B:90:THR:O	1:B:93:ASP:N	2.42	0.53
1:C:70:ILE:HD12	1:C:117:MET:HG2	1.90	0.53
1:D:122:ARG:HG2	1:D:128:VAL:HG12	1.89	0.53
1:B:108:VAL:HA	1:B:131:GLY:O	2.08	0.53
1:B:29:ILE:HG13	1:B:29:ILE:O	2.09	0.53
1:B:209:TYR:O	1:B:212:VAL:HG22	2.09	0.53
1:B:37:VAL:HB	1:B:215:VAL:HA	1.91	0.53
1:B:54:ASP:C	1:B:56:GLU:N	2.62	0.53
1:A:111:VAL:HG11	1:A:134:LEU:HD13	1.91	0.52
1:B:103:SER:HB2	1:B:159:TRP:CD1	2.44	0.52
1:D:221:ILE:HG23	1:D:230:VAL:O	2.08	0.52
1:D:148:TYR:CZ	1:D:150:LYS:HG3	2.45	0.52
1:B:160:VAL:CG1	1:B:190:ILE:HG12	2.40	0.52
1:B:220:ASP:HB3	1:B:231:PRO:HD2	1.92	0.52
1:B:44:GLN:O	1:B:48:MET:HG3	2.09	0.52
1:C:152:PRO:HG2	1:C:155:ILE:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:HG2	2:B:3699:PO4:O3	2.10	0.52
1:B:89:THR:HG23	1:C:55:LYS:HD3	1.92	0.51
1:A:64:PHE:CZ	1:D:126:ARG:HD2	2.45	0.51
1:A:90:THR:HG22	1:A:92:LEU:N	2.13	0.51
1:B:154:ASP:HB3	1:B:158:ARG:NH1	2.24	0.51
1:A:230:VAL:HA	1:A:231:PRO:C	2.30	0.51
1:C:59:LYS:HG3	1:C:60:GLU:H	1.74	0.51
1:B:104:LYS:HG2	1:B:158:ARG:HH21	1.75	0.51
1:A:222:CYS:O	1:A:230:VAL:HG22	2.11	0.51
1:D:156:ARG:HB2	1:D:156:ARG:NH1	2.26	0.51
1:B:111:VAL:HB	1:B:134:LEU:CD1	2.41	0.51
1:D:237:GLY:O	1:D:241:PHE:HD1	1.94	0.51
1:C:58:PRO:HG2	1:C:61:GLU:HB2	1.93	0.51
1:A:226:ARG:HD3	1:A:227:TYR:H	1.76	0.51
1:A:77:ALA:C	1:A:79:ASN:H	2.13	0.51
1:D:137:ARG:NH2	1:D:172:SER:HB3	2.25	0.51
1:D:30:ILE:HG22	1:D:31:THR:CG2	2.41	0.51
1:D:205:VAL:HG23	1:D:206:PHE:N	2.25	0.51
1:C:42:THR:O	1:C:46:ARG:HG2	2.11	0.51
1:A:79:ASN:OD1	1:D:44:GLN:HB2	2.10	0.51
1:B:133:ILE:HG22	1:B:135:ILE:HG13	1.93	0.50
1:B:196:LEU:HD13	1:B:229:ILE:CD1	2.41	0.50
1:D:200:GLN:NE2	1:D:223:LEU:HD13	2.26	0.50
1:C:160:VAL:CG1	1:C:190:ILE:HG12	2.41	0.50
1:A:117:MET:HG3	1:A:163:LEU:HG	1.93	0.50
1:B:85:LYS:HE2	1:B:97:HIS:HB3	1.93	0.50
1:C:173:VAL:O	1:C:177:ILE:HG13	2.12	0.50
1:D:145:LYS:HB3	1:D:145:LYS:NZ	2.27	0.50
1:D:242:GLY:N	6:D:767:HOH:O	2.44	0.50
1:B:112:ARG:HG3	1:A:148:TYR:OH	2.10	0.50
1:C:165:PRO:O	1:C:194:ASN:ND2	2.44	0.50
1:A:137:ARG:HG2	1:A:144:PRO:HA	1.93	0.50
1:D:229:ILE:O	1:D:232:GLY:HA3	2.12	0.50
1:B:129:ARG:HH11	1:B:158:ARG:HH22	1.60	0.50
1:C:41:GLN:HA	1:C:45:LEU:HD23	1.93	0.50
1:D:241:PHE:HA	6:D:767:HOH:O	2.12	0.49
1:D:104:LYS:HG2	2:D:3799:PO4:O2	2.11	0.49
1:B:223:LEU:HD12	1:B:229:ILE:HA	1.94	0.49
1:A:50:THR:CG2	1:D:98:GLY:HA3	2.42	0.49
1:C:219:VAL:HG13	1:C:219:VAL:O	2.12	0.49
1:C:66:ALA:O	1:C:70:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG23	1:B:64:PHE:N	2.27	0.49
1:C:90:THR:HG22	1:C:94:VAL:HG22	1.93	0.49
1:D:39:MET:CE	1:D:45:LEU:HD11	2.42	0.49
1:C:121:LEU:HD12	6:C:790:HOH:O	2.12	0.49
1:B:146:LEU:C	1:B:147:ILE:HD12	2.32	0.49
1:D:137:ARG:N	1:D:137:ARG:HH11	2.11	0.49
1:B:61:GLU:OE2	1:C:126:ARG:NH1	2.45	0.49
1:C:230:VAL:O	1:C:231:PRO:O	2.31	0.49
1:D:29:ILE:C	1:D:29:ILE:HD12	2.33	0.49
1:A:115:GLU:HA	1:A:118:GLU:HG3	1.94	0.49
1:C:28:ASP:O	1:C:32:ARG:HG3	2.12	0.49
1:B:90:THR:HG21	1:C:231:PRO:O	2.13	0.49
1:C:156:ARG:CD	1:C:156:ARG:H	2.12	0.49
1:C:201:GLY:O	1:C:205:VAL:HG13	2.13	0.49
1:C:53:ARG:HH21	1:C:232:GLY:N	2.11	0.48
1:A:224:ASN:O	1:A:226:ARG:O	2.30	0.48
1:C:224:ASN:HD21	1:C:228:TYR:H	1.61	0.48
1:C:181:LEU:C	1:C:183:LEU:H	2.17	0.48
1:A:48:MET:HE3	1:A:68:ARG:CG	2.41	0.48
1:A:133:ILE:HD11	1:A:151:LEU:HD21	1.96	0.48
1:B:77:ALA:CB	1:B:215:VAL:HG11	2.43	0.48
1:B:85:LYS:HZ1	1:B:87:GLU:HG3	1.78	0.48
1:D:224:ASN:HD22	1:D:224:ASN:C	2.16	0.48
1:B:70:ILE:CD1	1:B:195:ILE:HD11	2.44	0.48
1:A:166:MET:HG2	1:A:229:ILE:HD13	1.95	0.48
1:B:154:ASP:OD1	1:B:158:ARG:NH1	2.47	0.48
1:B:49:MET:O	1:B:53:ARG:HB2	2.13	0.48
1:D:104:LYS:CG	1:D:158:ARG:HH21	2.26	0.48
1:A:169:THR:HG23	2:A:1599:PO4:P	2.54	0.48
1:C:80:GLU:HB2	1:C:191:ILE:HD13	1.96	0.48
1:C:168:ALA:HB3	2:C:2599:PO4:O4	2.13	0.48
1:D:150:LYS:HD2	1:C:112:ARG:NE	2.28	0.48
1:B:173:VAL:HG21	1:B:192:PHE:CE1	2.49	0.48
1:B:213:ARG:NH1	1:B:213:ARG:HG2	2.28	0.48
1:D:74:ILE:O	1:D:78:LEU:HG	2.14	0.48
1:B:85:LYS:NZ	1:B:87:GLU:HG3	2.28	0.48
1:D:39:MET:HE3	1:D:45:LEU:HD11	1.96	0.48
1:C:70:ILE:HG23	1:C:117:MET:HG2	1.95	0.47
1:A:169:THR:O	1:A:170:ALA:HB3	2.14	0.47
1:A:117:MET:HG2	1:A:117:MET:H	1.47	0.47
1:C:224:ASN:HD22	1:C:224:ASN:C	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:GLN:O	1:D:25:ILE:HG12	2.15	0.47
1:A:48:MET:HE2	1:A:69:LEU:HB2	1.95	0.47
1:D:90:THR:C	1:D:92:LEU:H	2.18	0.47
1:A:111:VAL:HG21	1:A:134:LEU:HB2	1.96	0.47
1:C:69:LEU:HD23	1:C:195:ILE:HD12	1.95	0.47
1:A:57:THR:HA	1:A:58:PRO:HD3	1.72	0.47
1:A:111:VAL:CG1	1:A:134:LEU:HD13	2.45	0.47
1:C:105:ILE:HD13	1:C:105:ILE:H	1.77	0.47
1:D:105:ILE:HG22	1:D:159:TRP:HB2	1.97	0.47
1:C:105:ILE:N	1:C:105:ILE:HD13	2.30	0.47
1:A:26:LEU:HD12	1:A:219:VAL:CG1	2.45	0.47
1:D:49:MET:HE3	1:D:52:ILE:HG21	1.97	0.47
1:D:36:VAL:O	1:D:36:VAL:HG23	2.14	0.47
1:D:169:THR:O	1:D:170:ALA:HB3	2.14	0.47
1:D:136:GLN:HE22	1:C:148:TYR:HD2	1.63	0.47
1:C:200:GLN:HE22	1:C:223:LEU:HG	1.80	0.47
1:C:136:GLN:CB	1:C:147:ILE:HD11	2.44	0.47
1:C:190:ILE:HB	1:C:212:VAL:HG12	1.98	0.46
1:D:32:ARG:HG2	1:D:32:ARG:HH11	1.80	0.46
1:B:103:SER:HB2	1:B:159:TRP:NE1	2.30	0.46
1:C:53:ARG:HH21	1:C:232:GLY:CA	2.28	0.46
1:B:152:PRO:HA	1:A:243:THR:HG22	1.97	0.46
1:D:53:ARG:HH22	1:D:220:ASP:CG	2.18	0.46
1:D:37:VAL:HG13	1:D:215:VAL:HA	1.98	0.46
1:C:196:LEU:HD23	1:C:197:ALA:N	2.29	0.46
1:C:114:GLY:O	1:C:117:MET:N	2.45	0.46
1:B:52:ILE:O	1:B:62:PHE:HE1	1.99	0.46
1:B:23:GLU:O	1:B:27:GLN:HB2	2.16	0.46
1:A:175:LYS:O	1:A:175:LYS:HD3	2.15	0.46
1:B:169:THR:O	1:B:170:ALA:HB3	2.14	0.46
1:D:197:ALA:HB1	1:D:202:ILE:HD11	1.97	0.46
1:C:48:MET:CE	1:C:69:LEU:HB2	2.45	0.46
1:B:102:TYR:HD2	1:B:103:SER:H	1.64	0.46
1:C:233:ILE:O	1:C:233:ILE:CG2	2.64	0.46
1:C:62:PHE:C	1:C:62:PHE:CD1	2.89	0.46
1:D:70:ILE:O	1:D:73:LEU:N	2.46	0.46
1:A:165:PRO:O	1:A:194:ASN:ND2	2.49	0.45
1:D:197:ALA:HB1	1:D:202:ILE:CD1	2.46	0.45
1:B:132:LYS:HE3	1:A:112:ARG:HG3	1.98	0.45
1:D:155:ILE:O	1:D:158:ARG:HG3	2.16	0.45
1:D:49:MET:HA	1:D:52:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HG3	1:D:55:LYS:HB3	1.97	0.45
1:B:104:LYS:HE2	1:B:105:ILE:H	1.81	0.45
1:B:111:VAL:CB	1:B:134:LEU:HD13	2.46	0.45
1:A:226:ARG:HD3	1:A:227:TYR:N	2.31	0.45
1:C:161:MET:HE2	1:C:191:ILE:HD12	1.98	0.45
1:A:125:CYS:O	1:A:128:VAL:HB	2.16	0.45
1:A:133:ILE:HD13	1:A:149:GLU:HB2	1.98	0.45
1:B:241:PHE:HD2	1:A:130:ILE:HB	1.82	0.45
1:C:199:PRO:O	1:C:203:GLU:HG3	2.17	0.45
1:A:226:ARG:CG	1:A:227:TYR:H	2.30	0.45
1:D:108:VAL:HG23	1:D:160:VAL:HG13	1.98	0.45
1:A:126:ARG:O	1:A:128:VAL:N	2.49	0.45
1:C:102:TYR:HD2	1:C:102:TYR:H	1.60	0.45
1:C:136:GLN:HB2	1:C:147:ILE:CD1	2.47	0.45
1:A:59:LYS:HG2	1:A:60:GLU:OE1	2.16	0.45
1:B:104:LYS:HG2	1:B:158:ARG:NH2	2.32	0.45
1:A:160:VAL:HG23	1:A:190:ILE:HG12	1.99	0.45
1:A:53:ARG:NH2	1:A:220:ASP:OD2	2.50	0.45
1:A:158:ARG:HG2	1:A:158:ARG:H	1.68	0.45
1:D:60:GLU:N	1:D:60:GLU:CD	2.67	0.45
1:D:235:ASP:O	1:D:239:ARG:HG3	2.17	0.45
1:C:141:THR:HG22	1:C:143:GLU:OE2	2.17	0.45
1:C:115:GLU:HB2	6:C:825:HOH:O	2.18	0.44
1:A:149:GLU:O	1:A:149:GLU:HG3	2.16	0.44
1:A:160:VAL:HG21	1:A:185:VAL:HG21	1.98	0.44
1:C:197:ALA:O	1:C:219:VAL:HA	2.17	0.44
1:A:135:ILE:HD12	1:A:175:LYS:HB3	2.00	0.44
1:D:26:LEU:HD11	1:D:219:VAL:HB	1.99	0.44
1:A:82:PRO:HG2	1:A:103:SER:OG	2.17	0.44
1:B:235:ASP:CG	1:B:238:ASP:HB2	2.37	0.44
1:D:110:ILE:HD12	1:D:164:ASP:HB2	1.98	0.44
1:B:129:ARG:NH1	2:B:3699:PO4:O4	2.51	0.44
1:A:35:ASN:HB2	1:A:206:PHE:CE2	2.52	0.44
1:C:26:LEU:HD12	1:C:219:VAL:HG13	1.98	0.44
1:C:223:LEU:HD23	1:C:229:ILE:HA	1.99	0.44
1:D:186:LYS:HD3	1:D:186:LYS:N	2.32	0.44
1:A:48:MET:HE2	1:A:69:LEU:CA	2.47	0.44
1:D:70:ILE:O	1:D:73:LEU:HB2	2.17	0.44
1:C:102:TYR:N	1:C:102:TYR:CD2	2.83	0.44
1:D:226:ARG:HA	1:D:226:ARG:HD3	1.82	0.44
1:A:167:CYS:HB3	1:A:197:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:GLY:O	1:C:243:THR:C	2.56	0.44
1:A:37:VAL:HB	1:A:215:VAL:HG22	1.99	0.44
1:B:221:ILE:HG13	1:B:222:CYS:N	2.32	0.44
1:C:194:ASN:O	1:C:216:THR:HA	2.17	0.44
1:D:241:PHE:CA	6:D:767:HOH:O	2.65	0.44
1:A:184:GLY:O	1:A:185:VAL:C	2.54	0.44
1:B:235:ASP:CB	1:B:238:ASP:HB2	2.47	0.44
1:A:77:ALA:C	1:A:79:ASN:N	2.71	0.44
1:C:49:MET:CE	1:C:52:ILE:HD11	2.48	0.44
1:B:231:PRO:HA	1:C:94:VAL:HG21	2.00	0.44
1:C:62:PHE:O	1:C:66:ALA:HB2	2.18	0.44
1:B:134:LEU:HD23	1:B:147:ILE:HG22	2.00	0.44
1:D:115:GLU:OE1	1:C:115:GLU:OE1	2.36	0.43
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.83	0.43
1:C:113:ALA:N	6:C:825:HOH:O	2.51	0.43
1:A:111:VAL:HB	1:A:134:LEU:HD13	1.99	0.43
1:C:205:VAL:CG2	1:C:206:PHE:N	2.81	0.43
1:A:55:LYS:HE3	1:D:89:THR:OG1	2.17	0.43
1:C:110:ILE:CD1	1:C:162:LEU:HD11	2.41	0.43
1:D:122:ARG:NH2	1:C:241:PHE:HA	2.34	0.43
1:A:168:ALA:HB2	1:A:229:ILE:HD11	2.00	0.43
1:D:136:GLN:HB2	1:D:147:ILE:HG13	1.99	0.43
1:B:23:GLU:O	1:B:23:GLU:HG3	2.18	0.43
1:D:47:ALA:O	1:D:51:ILE:HG22	2.18	0.43
1:D:51:ILE:O	1:D:57:THR:HG21	2.19	0.43
1:B:44:GLN:HB2	1:C:79:ASN:OD1	2.19	0.43
1:C:224:ASN:ND2	1:C:224:ASN:C	2.72	0.43
1:C:33:PHE:CZ	1:C:203:GLU:HG2	2.54	0.43
1:D:63:VAL:O	1:D:64:PHE:C	2.57	0.43
1:C:48:MET:HE1	1:C:69:LEU:N	2.34	0.43
1:D:154:ASP:O	1:D:156:ARG:N	2.51	0.43
1:D:154:ASP:HB3	1:D:158:ARG:HD2	1.99	0.43
1:A:202:ILE:O	1:A:206:PHE:HD1	2.01	0.43
1:A:135:ILE:HG21	1:A:172:SER:HA	2.00	0.43
1:B:233:ILE:CD1	1:B:233:ILE:O	2.64	0.43
1:B:29:ILE:HD13	1:B:219:VAL:HG11	1.99	0.43
1:A:160:VAL:CG2	1:A:185:VAL:HG21	2.49	0.43
1:C:226:ARG:HB3	1:C:228:TYR:CD1	2.51	0.43
1:D:112:ARG:H	1:D:115:GLU:CG	2.22	0.43
1:D:154:ASP:OD1	1:D:158:ARG:NH1	2.51	0.43
1:A:35:ASN:HB2	1:A:206:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ILE:HG21	1:C:220:ASP:O	2.18	0.43
1:D:51:ILE:HG13	1:D:57:THR:CG2	2.33	0.43
1:C:44:GLN:O	1:C:48:MET:HG3	2.19	0.43
1:D:238:ASP:OD1	1:D:238:ASP:N	2.51	0.43
1:D:155:ILE:HA	1:D:158:ARG:HG3	2.01	0.43
1:C:187:GLU:OE1	1:C:209:TYR:HB3	2.18	0.43
1:B:91:PRO:C	1:B:93:ASP:H	2.21	0.42
1:D:242:GLY:O	1:D:243:THR:C	2.57	0.42
1:D:148:TYR:OH	1:D:150:LYS:HE2	2.19	0.42
1:B:117:MET:HE1	1:B:193:VAL:HG12	2.00	0.42
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.89	0.42
1:A:169:THR:N	2:A:1599:PO4:O1	2.52	0.42
1:B:222:CYS:SG	1:B:230:VAL:HG21	2.59	0.42
1:B:22:GLU:C	1:B:24:SER:N	2.72	0.42
1:C:114:GLY:HA2	1:C:165:PRO:HD3	2.01	0.42
1:B:62:PHE:HZ	1:B:233:ILE:HD11	1.82	0.42
1:C:233:ILE:HG23	1:C:239:ARG:NH1	2.34	0.42
1:A:132:LYS:O	1:A:133:ILE:HD13	2.19	0.42
1:C:58:PRO:O	1:C:59:LYS:C	2.58	0.42
1:B:132:LYS:HE2	1:A:241:PHE:CE2	2.54	0.42
1:A:188:GLU:HA	1:A:211:LYS:O	2.20	0.42
1:B:159:TRP:CE3	1:B:189:ARG:HG3	2.55	0.42
1:B:52:ILE:O	1:B:233:ILE:HG13	2.20	0.42
1:C:208:GLU:HG2	1:C:209:TYR:CE1	2.55	0.42
1:A:112:ARG:HB3	2:A:3599:PO4:O2	2.20	0.42
1:C:174:CYS:SG	1:C:204:ARG:HD3	2.59	0.42
1:D:129:ARG:HH12	2:D:3799:PO4:P	2.42	0.42
1:C:196:LEU:HD22	1:C:229:ILE:HG21	2.02	0.42
1:B:74:ILE:HD13	1:B:193:VAL:HG11	2.02	0.42
1:A:33:PHE:CE2	1:A:202:ILE:HD11	2.53	0.42
1:C:112:ARG:C	6:C:825:HOH:O	2.58	0.42
1:D:90:THR:CG2	1:D:94:VAL:HG13	2.49	0.42
1:B:166:MET:CE	1:B:236:PHE:HB2	2.50	0.42
1:C:72:LEU:HA	1:C:72:LEU:HD13	1.84	0.42
1:C:89:THR:HA	1:C:94:VAL:O	2.19	0.41
1:A:178:GLU:HB2	1:A:209:TYR:OH	2.18	0.41
1:C:117:MET:C	6:C:820:HOH:O	2.58	0.41
1:A:229:ILE:O	1:A:232:GLY:HA3	2.19	0.41
1:C:153:ALA:O	1:C:156:ARG:NH1	2.53	0.41
1:A:90:THR:HG23	1:A:91:PRO:HD2	2.02	0.41
1:D:154:ASP:HB3	1:D:158:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:O	1:A:147:ILE:HD13	2.20	0.41
1:C:74:ILE:HA	1:C:74:ILE:HD13	1.88	0.41
1:D:90:THR:HG23	1:D:92:LEU:N	2.32	0.41
1:A:159:TRP:CD1	1:A:189:ARG:HD3	2.55	0.41
1:B:44:GLN:HE22	1:B:68:ARG:HH22	1.69	0.41
1:A:111:VAL:CB	1:A:134:LEU:HD13	2.50	0.41
1:B:152:PRO:HD2	1:B:155:ILE:HD12	2.02	0.41
1:C:169:THR:O	1:C:170:ALA:HB3	2.19	0.41
1:D:26:LEU:O	1:D:30:ILE:HB	2.21	0.41
1:C:78:LEU:HD11	6:C:790:HOH:O	2.20	0.41
1:B:102:TYR:CD2	1:B:103:SER:N	2.87	0.41
1:B:141:THR:O	1:B:142:ALA:HB3	2.20	0.41
1:C:59:LYS:O	1:C:60:GLU:C	2.58	0.41
1:A:98:GLY:HA3	1:D:50:THR:OG1	2.20	0.41
1:B:158:ARG:NH2	2:B:3699:PO4:O4	2.54	0.41
1:C:74:ILE:HD13	1:C:193:VAL:HG11	2.02	0.41
1:A:50:THR:HG21	1:D:98:GLY:HA3	2.02	0.41
1:C:224:ASN:ND2	1:C:226:ARG:H	2.19	0.41
1:C:84:GLN:HG3	1:C:102:TYR:CE2	2.56	0.41
1:A:205:VAL:HG11	1:A:214:MET:CE	2.51	0.41
1:B:22:GLU:C	1:B:24:SER:H	2.24	0.41
1:C:181:LEU:O	1:C:183:LEU:N	2.53	0.41
1:B:33:PHE:N	1:B:34:PRO:HD3	2.35	0.41
1:C:70:ILE:HD13	1:C:195:ILE:HD11	2.02	0.41
1:B:196:LEU:HD22	1:B:197:ALA:H	1.84	0.41
1:B:166:MET:HG2	4:B:300:URA:C4	2.56	0.41
1:A:211:LYS:N	6:A:795:HOH:O	2.34	0.41
1:C:166:MET:HE3	1:C:229:ILE:HD12	2.03	0.41
1:B:228:TYR:HA	4:B:300:URA:H5	1.86	0.41
1:D:126:ARG:HG3	1:D:126:ARG:H	1.55	0.41
1:B:26:LEU:HD11	1:B:38:LEU:HG	2.03	0.41
1:B:107:GLY:O	1:B:130:ILE:HA	2.20	0.41
1:D:233:ILE:HD12	1:D:233:ILE:O	2.21	0.40
1:C:179:VAL:O	1:C:183:LEU:HG	2.21	0.40
1:C:135:ILE:HG22	1:C:136:GLN:N	2.37	0.40
1:A:98:GLY:CA	1:D:50:THR:OG1	2.69	0.40
1:A:154:ASP:CA	1:A:156:ARG:HH11	2.35	0.40
1:B:202:ILE:HG13	1:B:214:MET:HE3	2.01	0.40
1:B:63:VAL:CG2	1:B:64:PHE:N	2.85	0.40
1:A:85:LYS:HZ1	1:A:97:HIS:HB3	1.87	0.40
1:A:226:ARG:HG3	1:A:227:TYR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HD13	1:C:30:ILE:HA	1.90	0.40
1:C:224:ASN:ND2	1:C:228:TYR:H	2.18	0.40
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.95	0.40
1:A:148:TYR:O	1:A:149:GLU:HB3	2.22	0.40
1:B:78:LEU:HD23	1:B:161:MET:CE	2.52	0.40
1:D:209:TYR:O	1:D:212:VAL:HG22	2.22	0.40
1:A:158:ARG:HH22	2:A:3199:PO4:P	2.45	0.40
1:B:35:ASN:HB2	1:B:206:PHE:CE1	2.57	0.40
1:A:70:ILE:HD11	1:A:195:ILE:HD11	2.02	0.40
1:D:36:VAL:HG12	1:D:206:PHE:CE2	2.57	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	215/243 (88%)	187 (87%)	23 (11%)	5 (2%)	8	12
1	B	222/243 (91%)	191 (86%)	27 (12%)	4 (2%)	11	18
1	C	221/243 (91%)	183 (83%)	33 (15%)	5 (2%)	8	12
1	D	215/243 (88%)	185 (86%)	22 (10%)	8 (4%)	4	5
All	All	873/972 (90%)	746 (86%)	105 (12%)	22 (2%)	7	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	155	ILE
1	C	220	ASP
1	C	232	GLY
1	B	103	SER
1	B	112	ARG

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Mol	Chain	Res	Type
1	B	155	ILE
1	A	127	GLY
1	A	185	VAL
1	D	59	LYS
1	D	103	SER
1	C	60	GLU
1	C	182	ARG
1	B	168	ALA
1	A	111	VAL
1	A	126	ARG
1	C	59	LYS
1	D	156	ARG
1	D	112	ARG
1	D	91	PRO
1	A	210	PRO
1	D	111	VAL
1	D	231	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	192/212 (91%)	165 (86%)	27 (14%)	4	7
1	B	196/212 (92%)	174 (89%)	22 (11%)	7	14
1	C	195/212 (92%)	177 (91%)	18 (9%)	11	21
1	D	192/212 (91%)	171 (89%)	21 (11%)	8	15
All	All	775/848 (91%)	687 (89%)	88 (11%)	7	13

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	MET
1	B	51	ILE
1	B	57	THR
1	B	81	LEU

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Mol	Chain	Res	Type
1	B	92	LEU
1	B	94	VAL
1	B	104	LYS
1	B	112	ARG
1	B	117	MET
1	B	126	ARG
1	B	132	LYS
1	B	150	LYS
1	B	166	MET
1	B	180	LEU
1	B	188	GLU
1	B	189	ARG
1	B	194	ASN
1	B	196	LEU
1	B	213	ARG
1	B	226	ARG
1	B	233	ILE
1	B	238	ASP
1	A	23	GLU
1	A	29	ILE
1	A	50	THR
1	A	57	THR
1	A	61	GLU
1	A	72	LEU
1	A	79	ASN
1	A	91	PRO
1	A	92	LEU
1	A	108	VAL
1	A	117	MET
1	A	138	ASP
1	A	143	GLU
1	A	149	GLU
1	A	155	ILE
1	A	156	ARG
1	A	158	ARG
1	A	160	VAL
1	A	163	LEU
1	A	166	MET
1	A	169	THR
1	A	175	LYS
1	A	182	ARG
1	A	188	GLU

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	202	ILE
1	A	204	ARG
1	D	30	ILE
1	D	32	ARG
1	D	38	LEU
1	D	49	MET
1	D	56	GLU
1	D	60	GLU
1	D	73	LEU
1	D	81	LEU
1	D	94	VAL
1	D	156	ARG
1	D	158	ARG
1	D	163	LEU
1	D	166	MET
1	D	178	GLU
1	D	196	LEU
1	D	204	ARG
1	D	213	ARG
1	D	221	ILE
1	D	224	ASN
1	D	233	ILE
1	D	238	ASP
1	C	50	THR
1	C	69	LEU
1	C	90	THR
1	C	104	LYS
1	C	105	ILE
1	C	136	GLN
1	C	149	GLU
1	C	156	ARG
1	C	158	ARG
1	C	163	LEU
1	C	188	GLU
1	C	192	PHE
1	C	196	LEU
1	C	204	ARG
1	C	208	GLU
1	C	221	ILE
1	C	224	ASN
1	C	226	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	ASN
1	B	41	GLN
1	B	44	GLN
1	B	79	ASN
1	A	44	GLN
1	A	84	GLN
1	A	97	HIS
1	A	200	GLN
1	D	79	ASN
1	D	84	GLN
1	D	200	GLN
1	D	224	ASN
1	C	79	ASN
1	C	224	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	PO4	A	1599	-	4,4,4	1.27	0	6,6,6	0.27	0
2	PO4	A	3199	-	4,4,4	0.90	0	6,6,6	0.27	0
2	PO4	A	3599	-	4,4,4	0.77	0	6,6,6	0.27	0
4	URA	A	400	-	4,8,8	2.45	2 (50%)	6,10,10	12.15	4 (66%)
4	URA	B	300	-	4,8,8	2.85	2 (50%)	6,10,10	12.52	4 (66%)
5	PRP	B	301	3	19,22,22	2.57	6 (31%)	31,35,35	1.64	5 (16%)
2	PO4	B	3699	-	4,4,4	0.98	0	6,6,6	0.27	0
2	PO4	C	2599	-	4,4,4	1.01	0	6,6,6	0.27	0
2	PO4	C	3299	-	4,4,4	0.67	0	6,6,6	0.27	0
4	URA	C	600	-	4,8,8	2.50	2 (50%)	6,10,10	12.09	4 (66%)
2	PO4	D	3399	-	4,4,4	0.78	0	6,6,6	0.27	0
2	PO4	D	3499	-	4,4,4	0.98	0	6,6,6	0.27	0
2	PO4	D	3799	-	4,4,4	0.98	0	6,6,6	0.27	0
4	URA	D	500	-	4,8,8	2.42	2 (50%)	6,10,10	12.05	4 (66%)

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	PO4	A	1599	-	-	0/0/0/0	0/0/0/0
2	PO4	A	3199	-	-	0/0/0/0	0/0/0/0
2	PO4	A	3599	-	-	0/0/0/0	0/0/0/0
4	URA	A	400	-	-	0/0/0/0	0/1/1/1
4	URA	B	300	-	-	0/0/0/0	0/1/1/1
5	PRP	B	301	3	-	0/16/33/33	0/1/1/1
2	PO4	B	3699	-	-	0/0/0/0	0/0/0/0
2	PO4	C	2599	-	-	0/0/0/0	0/0/0/0
2	PO4	C	3299	-	-	0/0/0/0	0/0/0/0
4	URA	C	600	-	-	0/0/0/0	0/1/1/1
2	PO4	D	3399	-	-	0/0/0/0	0/0/0/0
2	PO4	D	3499	-	-	0/0/0/0	0/0/0/0
2	PO4	D	3799	-	-	0/0/0/0	0/0/0/0
4	URA	D	500	-	-	0/0/0/0	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	PRP	P-O5	-2.86	1.50	1.60
5	B	301	PRP	C1-C2	2.45	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	URA	C6-N1	2.55	1.40	1.34
4	D	500	URA	C6-N1	2.78	1.40	1.34
4	C	600	URA	C6-N1	2.86	1.40	1.34
5	B	301	PRP	O3-C3	3.12	1.50	1.43
4	B	300	URA	C6-N1	3.35	1.41	1.34
4	D	500	URA	C4-N3	3.66	1.39	1.33
4	A	400	URA	C4-N3	3.81	1.40	1.33
4	C	600	URA	C4-N3	3.91	1.40	1.33
5	B	301	PRP	P-O3P	4.16	1.69	1.54
4	B	300	URA	C4-N3	4.35	1.41	1.33
5	B	301	PRP	PA-O1	4.73	1.73	1.60
5	B	301	PRP	O4-C1	6.53	1.53	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	300	URA	N1-C2-N3	-22.40	114.04	128.33
4	A	400	URA	N1-C2-N3	-21.76	114.45	128.33
4	C	600	URA	N1-C2-N3	-21.73	114.47	128.33
4	D	500	URA	N1-C2-N3	-21.46	114.64	128.33
4	A	400	URA	C5-C4-N3	-3.12	115.12	123.12
4	C	600	URA	C5-C4-N3	-3.06	115.27	123.12
4	D	500	URA	C5-C4-N3	-2.88	115.72	123.12
4	B	300	URA	C5-C4-N3	-2.87	115.76	123.12
5	B	301	PRP	C2-C3-C4	-2.75	96.97	102.61
5	B	301	PRP	O4-C1-C2	-2.47	101.32	104.78
5	B	301	PRP	C1-C2-C3	3.75	107.50	102.45
5	B	301	PRP	O2A-PA-O3A	4.14	123.89	105.09
5	B	301	PRP	O1-C1-C2	4.15	114.06	106.67
4	A	400	URA	C4-N3-C2	12.86	126.88	114.14
4	D	500	URA	C4-N3-C2	13.00	127.02	114.14
4	C	600	URA	C4-N3-C2	13.27	127.28	114.14
4	B	300	URA	C4-N3-C2	13.43	127.44	114.14
4	C	600	URA	C6-N1-C2	14.75	121.66	114.40
4	D	500	URA	C6-N1-C2	15.17	121.86	114.40
4	A	400	URA	C6-N1-C2	15.31	121.93	114.40
4	B	300	URA	C6-N1-C2	15.77	122.16	114.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1599	PO4	2	0
2	A	3199	PO4	1	0
2	A	3599	PO4	1	0
4	B	300	URA	6	0
5	B	301	PRP	1	0
2	B	3699	PO4	4	0
2	C	2599	PO4	3	0
4	C	600	URA	1	0
2	D	3799	PO4	4	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, 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	219/243 (90%)	-0.01	0 100 100	29, 51, 77, 94	1 (0%)
1	B	224/243 (92%)	0.22	6 (2%) 58 62	35, 55, 83, 95	1 (0%)
1	C	223/243 (91%)	0.18	7 (3%) 52 57	35, 56, 83, 95	1 (0%)
1	D	219/243 (90%)	0.15	5 (2%) 64 67	31, 55, 83, 94	1 (0%)
All	All	885/972 (91%)	0.13	18 (2%) 68 72	29, 55, 83, 95	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	VAL	5.4
1	B	223	LEU	4.2
1	C	168	ALA	4.0
1	B	196	LEU	3.4
1	C	22	GLU	3.4
1	B	229	ILE	3.3
1	C	229	ILE	3.1
1	C	230	VAL	2.9
1	B	29	ILE	2.9
1	B	138	ASP	2.7
1	C	142	ALA	2.7
1	C	202	ILE	2.5
1	D	25	ILE	2.5
1	D	130	ILE	2.4
1	C	102	TYR	2.4
1	D	191	ILE	2.3
1	D	121	LEU	2.2
1	D	137	ARG	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	A	3599	5/5	0.93	0.32	4.92	67,68,69,70	0
5	PRP	B	301	22/22	0.85	0.28	3.95	27,38,52,61	0
4	URA	B	300	8/8	0.93	0.33	2.11	38,41,44,46	0
2	PO4	D	3399	5/5	0.93	0.19	0.41	65,68,70,71	0
4	URA	C	600	8/8	0.92	0.21	0.15	72,72,73,73	0
4	URA	A	400	8/8	0.92	0.16	-0.32	60,61,62,62	0
2	PO4	C	2599	5/5	0.95	0.10	-0.83	62,64,65,65	0
2	PO4	A	1599	5/5	0.98	0.11	-0.98	59,64,64,66	0
2	PO4	D	3499	5/5	0.98	0.07	-1.50	64,65,67,68	0
4	URA	D	500	8/8	0.93	0.09	-1.63	54,55,57,59	0
2	PO4	B	3699	5/5	0.93	0.11	-2.92	67,67,68,68	0
3	MG	B	3756	1/1	0.92	0.39	-	45,45,45,45	0
2	PO4	A	3199	5/5	0.95	0.07	-	66,68,69,70	0
2	PO4	C	3299	5/5	0.85	0.41	-	70,71,74,75	0
2	PO4	D	3799	5/5	0.96	0.12	-	66,66,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.