



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:37 am GMT

PDB ID : 3G1H
Title : Crystal structure of orotidine 5'-monophosphate decarboxylase from Methanobacterium thermoautotrophicum complexed with 5,6-dihydrouridine 5'-monophosphate
Authors : Fedorov, A.A.; Fedorov, E.V.; Chan, K.K.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2009-01-29
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

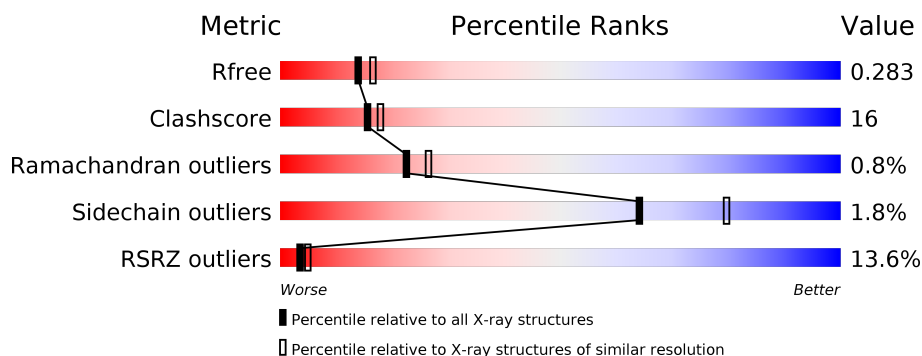
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	228	<div> <div>6%</div> <div>78% 19% .</div> </div>
1	B	228	<div> <div>8%</div> <div>69% 24% . 5%</div> </div>
1	C	228	<div> <div>6%</div> <div>73% 22% . .</div> </div>
1	D	228	<div> <div>9%</div> <div>65% 28% . 6%</div> </div>
1	E	228	<div> <div>13%</div> <div>67% 29% 5%</div> </div>
1	F	228	<div> <div>12%</div> <div>68% 27% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	228	<div><div></div><div>13%</div><div>59%</div><div>35%</div><div>• 5%</div></div>
1	H	228	<div><div></div><div>11%</div><div>65%</div><div>29%</div><div>• 5%</div></div>
1	I	228	<div><div></div><div>20%</div><div>60%</div><div>29%</div><div>• 7%</div></div>
1	J	228	<div><div></div><div>7%</div><div>70%</div><div>24%</div><div>• •</div></div>
1	K	228	<div><div></div><div>24%</div><div>60%</div><div>34%</div><div>• 5%</div></div>
1	L	228	<div><div></div><div>20%</div><div>57%</div><div>36%</div><div>• 5%</div></div>
1	M	228	<div><div></div><div>18%</div><div>74%</div><div>19%</div><div>• 5%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21877 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1679	1054	295	318	12			
1	B	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	C	218	Total	C	N	O	S	0	0	0
			1653	1039	289	313	12			
1	D	215	Total	C	N	O	S	0	0	0
			1630	1025	286	308	11			
1	E	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			
1	F	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			
1	G	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			
1	H	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	I	212	Total	C	N	O	S	0	0	0
			1607	1011	282	304	10			
1	J	218	Total	C	N	O	S	0	0	0
			1653	1039	289	313	12			
1	K	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	L	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	M	217	Total	C	N	O	S	0	0	0
			1646	1034	288	312	12			

There are 13 discrepancies between the modelled and reference sequences:

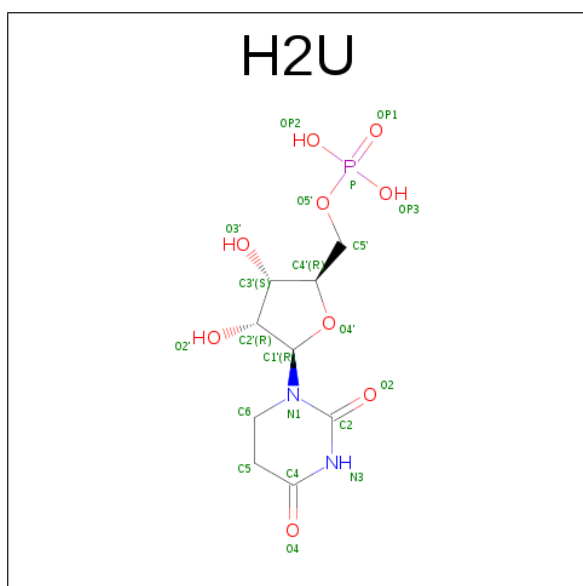
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	PRO	ARG	ENGINEERED	UNP O26232
B	101	PRO	ARG	ENGINEERED	UNP O26232
C	101	PRO	ARG	ENGINEERED	UNP O26232

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Chain	Residue	Modelled	Actual	Comment	Reference
D	101	PRO	ARG	ENGINEERED	UNP O26232
E	101	PRO	ARG	ENGINEERED	UNP O26232
F	101	PRO	ARG	ENGINEERED	UNP O26232
G	101	PRO	ARG	ENGINEERED	UNP O26232
H	101	PRO	ARG	ENGINEERED	UNP O26232
I	101	PRO	ARG	ENGINEERED	UNP O26232
J	101	PRO	ARG	ENGINEERED	UNP O26232
K	101	PRO	ARG	ENGINEERED	UNP O26232
L	101	PRO	ARG	ENGINEERED	UNP O26232
M	101	PRO	ARG	ENGINEERED	UNP O26232

- Molecule 2 is 5,6-DIHYDROURIDINE-5'-MONOPHOSPHATE (three-letter code: H2U) (formula: $C_9H_{15}N_2O_9P$).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	H	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	I	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	J	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	K	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	L	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	M	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

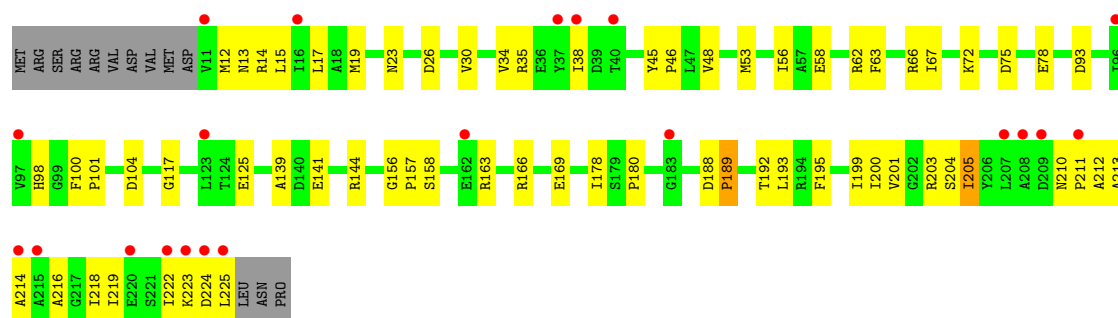
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	26	Total	O	0	0
			26	26		
3	C	44	Total	O	0	0
			44	44		
3	D	26	Total	O	0	0
			26	26		
3	E	9	Total	O	0	0
			9	9		
3	F	10	Total	O	0	0
			10	10		
3	G	7	Total	O	0	0
			7	7		
3	H	3	Total	O	0	0
			3	3		
3	I	14	Total	O	0	0
			14	14		
3	J	27	Total	O	0	0
			27	27		
3	K	4	Total	O	0	0
			4	4		
3	L	1	Total	O	0	0
			1	1		

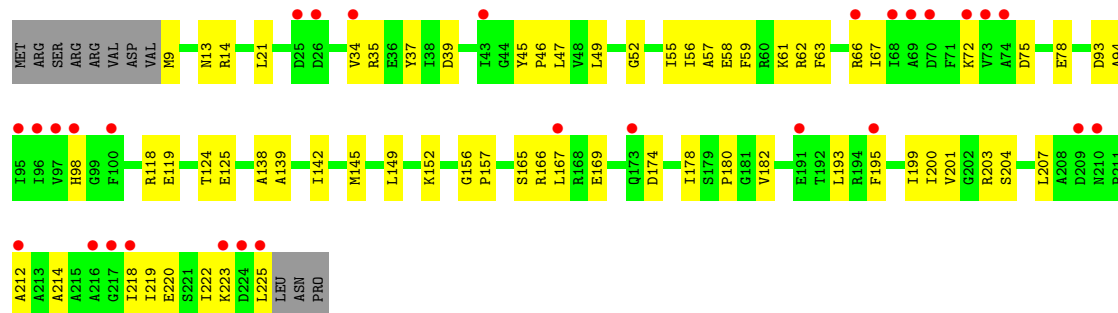
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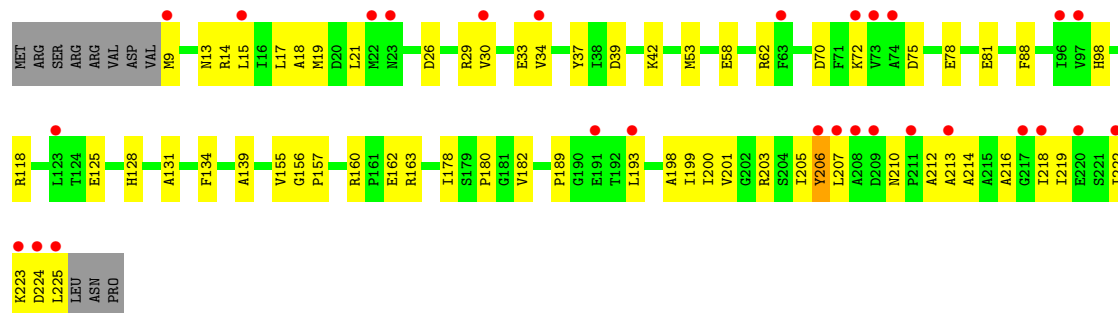
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	30	Total	O	0	0
			30	30		



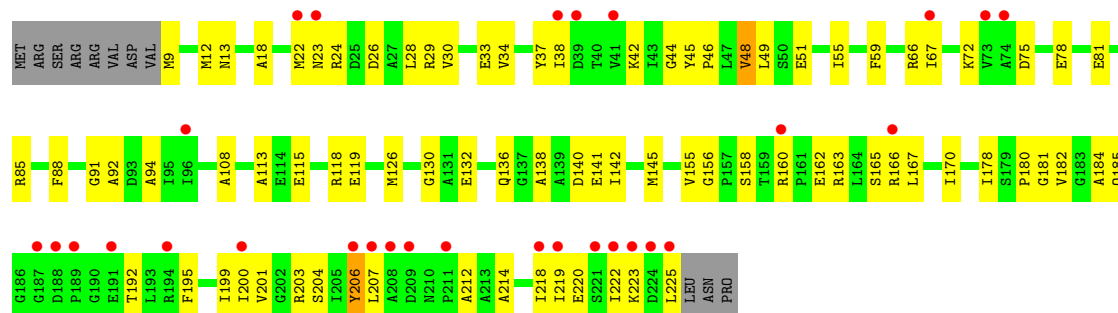
• Molecule 1: Orotidine 5'-phosphate decarboxylase



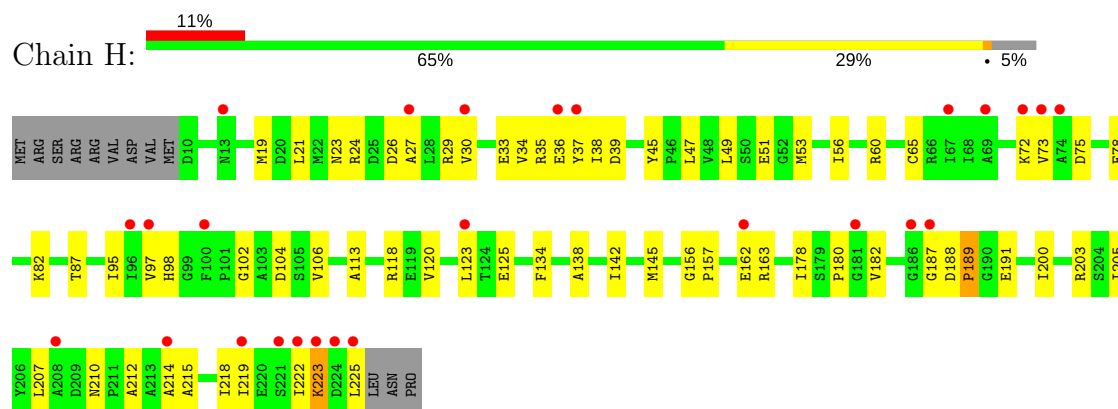
• Molecule 1: Orotidine 5'-phosphate decarboxylase



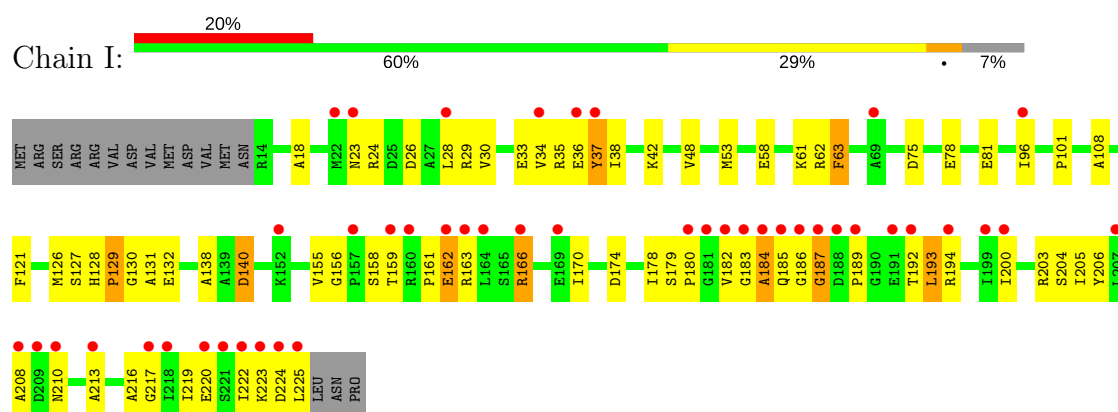
• Molecule 1: Orotidine 5'-phosphate decarboxylase



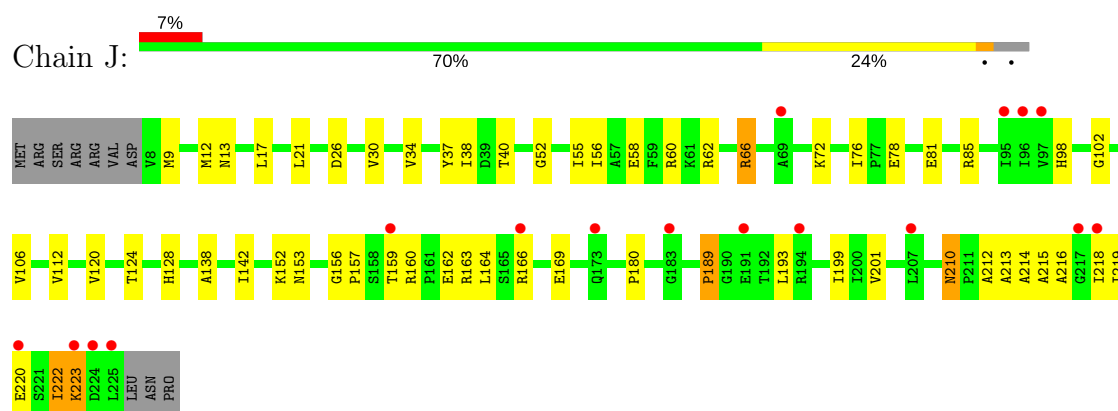
• Molecule 1: Orotidine 5'-phosphate decarboxylase



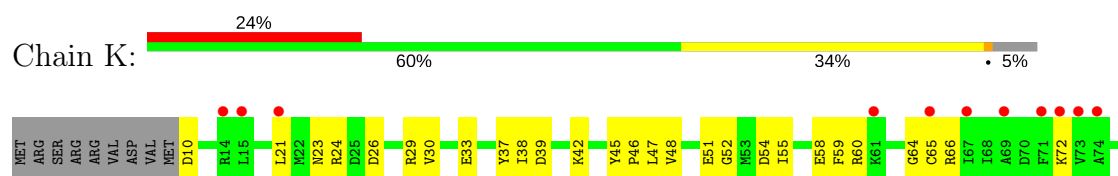
• Molecule 1: Orotidine 5'-phosphate decarboxylase

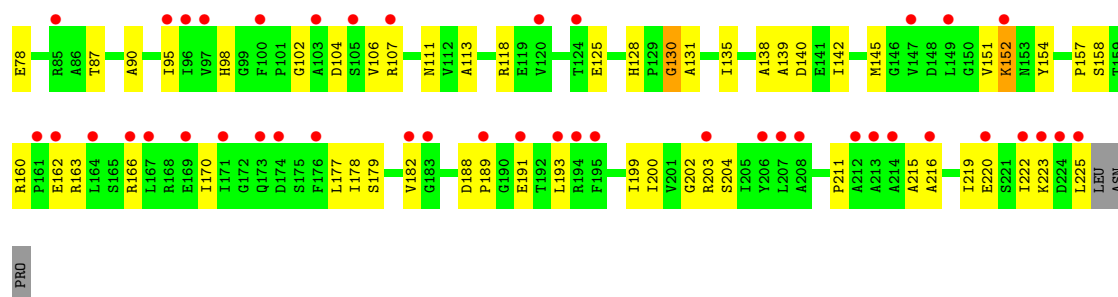


• Molecule 1: Orotidine 5'-phosphate decarboxylase

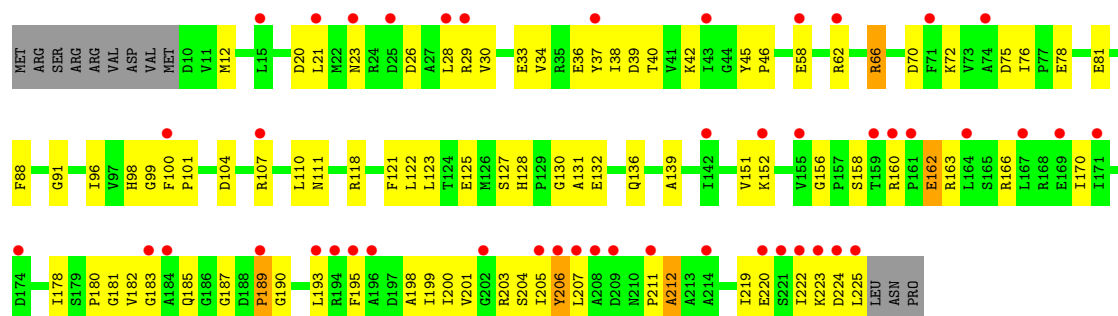


• Molecule 1: Orotidine 5'-phosphate decarboxylase

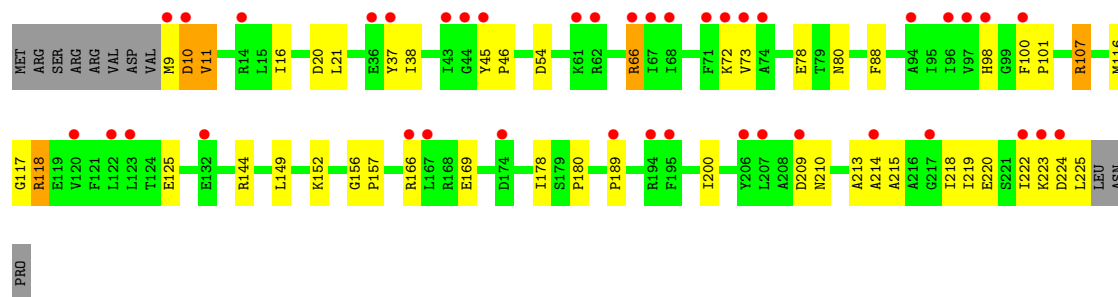
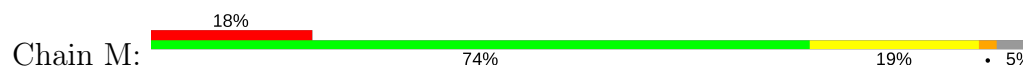




- Molecule 1: Orotidine 5'-phosphate decarboxylase



- Molecule 1: Orotidine 5'-phosphate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.90Å 101.80Å 192.83Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	24.76 – 2.30 39.92 – 2.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.76-2.30) 96.7 (39.92-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.285 0.242 , 0.283	Depositor DCC
R_{free} test set	6367 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21877	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: H2U

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/1702	0.70	1/2296 (0.0%)
1	B	0.48	1/1661 (0.1%)	0.63	0/2241
1	C	0.45	0/1676	0.65	0/2261
1	D	0.42	0/1653	0.62	0/2230
1	E	0.34	0/1669	0.58	0/2251
1	F	0.38	0/1669	0.60	0/2251
1	G	0.33	0/1669	0.57	0/2251
1	H	0.34	0/1661	0.56	0/2241
1	I	0.34	0/1630	0.59	0/2199
1	J	0.38	0/1676	0.60	0/2261
1	K	0.30	0/1661	0.52	0/2241
1	L	0.30	0/1661	0.52	0/2241
1	M	0.53	1/1669 (0.1%)	1.27	6/2251 (0.3%)
All	All	0.40	2/21657 (0.0%)	0.67	7/29215 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	CYS	CB-SG	7.00	1.94	1.82
1	M	11	VAL	CB-CG2	5.01	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	144	ARG	NE-CZ-NH1	-29.35	105.63	120.30
1	M	66	ARG	CA-CB-CG	26.22	171.07	113.40
1	M	144	ARG	NE-CZ-NH2	24.90	132.75	120.30
1	M	118	ARG	CG-CD-NE	18.51	150.67	111.80
1	M	144	ARG	CD-NE-CZ	13.57	142.60	123.60
1	M	144	ARG	CG-CD-NE	-7.40	96.26	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	LEU	CA-CB-CG	5.84	128.73	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1679	0	1695	36	0
1	B	1638	0	1651	54	0
1	C	1653	0	1669	48	0
1	D	1630	0	1647	60	0
1	E	1646	0	1660	53	0
1	F	1646	0	1660	55	0
1	G	1646	0	1660	75	0
1	H	1638	0	1651	53	0
1	I	1607	0	1623	75	0
1	J	1653	0	1669	55	0
1	K	1638	0	1651	67	1
1	L	1638	0	1651	84	0
1	M	1646	0	1660	44	0
2	A	21	0	13	0	0
2	B	21	0	13	0	0
2	C	21	0	13	1	0
2	D	21	0	13	2	0
2	E	21	0	13	0	0
2	F	21	0	13	1	0
2	G	21	0	13	1	0
2	H	21	0	13	0	0
2	I	21	0	13	2	0
2	J	21	0	13	0	0
2	K	21	0	13	0	0
2	L	21	0	13	0	0
2	M	21	0	13	2	0
3	A	45	0	0	0	0
3	B	26	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	0	2	0
3	D	26	0	0	1	0
3	E	9	0	0	2	0
3	F	10	0	0	0	0
3	G	7	0	0	0	0
3	H	3	0	0	1	0
3	I	14	0	0	3	0
3	J	27	0	0	1	0
3	K	4	0	0	0	0
3	L	1	0	0	0	0
3	M	30	0	0	5	0
All	All	21877	0	21716	713	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 16.

All (713) 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:M:116:MET:HE2	3:M:248:HOH:O	1.40	1.18
1:J:58:GLU:HG2	1:J:62:ARG:HD2	1.43	0.99
1:B:23:ASN:HD22	1:B:26:ASP:H	1.05	0.98
1:A:5:ARG:HG3	1:A:6:VAL:H	1.30	0.96
1:K:189:PRO:HB3	1:K:222:ILE:HD11	1.52	0.91
1:B:23:ASN:ND2	1:B:26:ASP:H	1.67	0.90
1:F:34:VAL:HG12	1:F:212:ALA:HA	1.57	0.86
1:G:222:ILE:HG23	1:G:225:LEU:HD12	1.56	0.85
1:G:34:VAL:HG12	1:G:212:ALA:HA	1.59	0.84
1:M:116:MET:CE	3:M:248:HOH:O	2.11	0.82
1:H:163:ARG:HH11	1:H:163:ARG:HA	1.45	0.81
1:I:156:GLY:O	1:I:180:PRO:HD2	1.80	0.81
1:J:163:ARG:HA	1:J:163:ARG:HH11	1.47	0.80
1:C:15:LEU:HD22	1:C:38:ILE:HG21	1.63	0.80
1:E:78:GLU:HG2	1:F:203:ARG:HH12	1.48	0.78
1:H:189:PRO:HB3	1:H:222:ILE:HD11	1.66	0.78
1:I:155:VAL:HG22	1:I:178:ILE:HD11	1.67	0.78
1:M:9:MET:HG3	1:M:9:MET:O	1.84	0.77
1:M:189:PRO:HB3	1:M:222:ILE:HD11	1.66	0.77
1:E:78:GLU:HG2	1:F:203:ARG:NH1	1.99	0.76
1:I:61:LYS:HD2	3:I:247:HOH:O	1.84	0.76
1:H:73:VAL:HB	1:H:97:VAL:HG13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:ILE:HG22	1:J:223:LYS:NZ	2.02	0.74
1:A:37:TYR:HB3	1:A:219:ILE:CD1	2.15	0.74
1:F:131:ALA:HB3	1:F:160:ARG:HH22	1.53	0.74
1:G:26:ASP:HA	1:G:29:ARG:HH12	1.52	0.73
1:G:220:GLU:OE1	1:G:223:LYS:HD3	1.88	0.73
1:I:220:GLU:OE1	1:I:223:LYS:HD3	1.88	0.73
1:H:205:ILE:HD11	1:H:218:ILE:HD12	1.70	0.73
1:K:26:ASP:HA	1:K:29:ARG:NH1	2.04	0.73
1:I:183:GLY:HA3	1:I:204:SER:OG	1.89	0.72
1:D:30:VAL:HG13	1:D:211:PRO:HB3	1.70	0.72
1:E:203:ARG:NH1	1:F:78:GLU:HG2	2.05	0.72
1:K:72:LYS:HB3	1:K:98:HIS:CD2	2.24	0.72
1:B:210:ASN:ND2	1:B:213:ALA:HB2	2.04	0.72
1:B:189:PRO:HB3	1:B:222:ILE:HD11	1.71	0.72
1:E:203:ARG:HH12	1:F:78:GLU:HG2	1.54	0.72
1:A:5:ARG:CG	1:A:6:VAL:H	2.02	0.72
1:I:219:ILE:O	1:I:223:LYS:HG3	1.90	0.72
1:K:26:ASP:HA	1:K:29:ARG:HH12	1.55	0.72
1:B:23:ASN:HD22	1:B:26:ASP:N	1.84	0.71
1:I:189:PRO:HB3	1:I:222:ILE:HD11	1.70	0.71
1:I:162:GLU:HA	3:I:230:HOH:O	1.89	0.71
1:B:33:GLU:HG3	3:B:239:HOH:O	1.89	0.71
1:H:163:ARG:NH1	1:H:163:ARG:HA	2.05	0.71
1:D:178:ILE:HD12	1:D:200:ILE:HD11	1.72	0.71
1:H:35:ARG:NH1	1:H:39:ASP:HA	2.06	0.71
1:M:220:GLU:OE1	1:M:223:LYS:HD3	1.92	0.70
1:G:115:GLU:HG2	1:G:115:GLU:O	1.89	0.70
1:L:201:VAL:HG13	1:L:204:SER:HB2	1.73	0.70
1:D:125:GLU:HB3	1:D:157:PRO:HD3	1.73	0.70
1:K:102:GLY:O	1:K:106:VAL:HG23	1.91	0.69
1:H:156:GLY:O	1:H:180:PRO:HD2	1.92	0.69
1:K:10:ASP:HB3	1:K:66:ARG:HH12	1.57	0.69
1:G:178:ILE:HD12	1:G:200:ILE:HD11	1.73	0.69
1:F:37:TYR:HB3	1:F:219:ILE:HD11	1.73	0.69
1:D:144:ARG:HH12	1:D:166:ARG:NH2	1.91	0.69
1:G:26:ASP:HA	1:G:29:ARG:NH1	2.08	0.68
1:I:184:ALA:HB1	1:I:203:ARG:HE	1.58	0.68
1:J:220:GLU:HA	1:J:223:LYS:HG2	1.75	0.68
1:M:210:ASN:ND2	1:M:213:ALA:HB2	2.08	0.68
1:B:23:ASN:HB3	1:B:26:ASP:HB2	1.74	0.68
1:L:180:PRO:HB3	1:L:200:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:ASP:OD2	1:M:11:VAL:O	2.09	0.68
1:A:37:TYR:HB3	1:A:219:ILE:HD12	1.75	0.68
1:G:166:ARG:O	1:G:170:ILE:HG13	1.94	0.68
1:E:35:ARG:NH1	1:E:39:ASP:HA	2.08	0.68
1:H:178:ILE:HD12	1:H:200:ILE:HD11	1.75	0.67
1:L:203:ARG:HB3	1:L:207:LEU:HD12	1.77	0.67
1:F:223:LYS:C	1:F:225:LEU:H	1.97	0.67
1:I:48:VAL:HG11	1:I:53:MET:SD	2.34	0.67
1:D:205:ILE:HD11	1:D:218:ILE:HD12	1.75	0.67
1:M:219:ILE:O	1:M:223:LYS:HG3	1.94	0.67
1:E:9:MET:HB2	3:E:249:HOH:O	1.93	0.67
1:B:210:ASN:HD22	1:B:213:ALA:HB2	1.60	0.66
1:H:182:VAL:HA	1:H:187:GLY:HA3	1.76	0.66
1:H:38:ILE:HD12	1:H:38:ILE:O	1.96	0.66
1:I:180:PRO:HB3	1:I:200:ILE:HD12	1.76	0.66
1:G:49:LEU:HD22	1:H:53:MET:SD	2.36	0.66
1:B:178:ILE:HD12	1:B:200:ILE:HD11	1.76	0.66
1:G:113:ALA:HB1	1:G:118:ARG:O	1.95	0.65
1:I:158:SER:HB2	1:I:179:SER:C	2.17	0.65
1:J:37:TYR:CZ	1:J:216:ALA:HB2	2.31	0.65
1:K:104:ASP:OD1	1:L:130:GLY:HA3	1.96	0.65
1:J:38:ILE:HD12	1:J:40:THR:O	1.96	0.65
1:L:152:LYS:HB3	1:L:152:LYS:NZ	2.12	0.65
1:L:21:LEU:HD23	1:L:26:ASP:HB3	1.79	0.64
1:H:182:VAL:HG13	1:H:187:GLY:O	1.97	0.64
1:I:58:GLU:O	1:I:62:ARG:HG2	1.97	0.64
1:F:58:GLU:O	1:F:62:ARG:HB2	1.97	0.64
1:J:124:THR:HG22	1:J:142:ILE:HG22	1.78	0.64
1:M:10:ASP:OD2	1:M:11:VAL:N	2.31	0.64
1:C:110:LEU:HD21	1:C:151:VAL:HG22	1.79	0.64
1:I:180:PRO:HA	1:I:200:ILE:HB	1.79	0.63
1:G:24:ARG:HB2	1:G:51:GLU:HG3	1.79	0.63
1:J:81:GLU:HG3	1:J:112:VAL:CG2	2.28	0.63
1:C:210:ASN:HD22	1:C:213:ALA:HB2	1.63	0.63
1:L:201:VAL:CG1	1:L:204:SER:HB2	2.29	0.63
1:L:34:VAL:HG13	1:L:211:PRO:O	1.99	0.63
1:H:37:TYR:HB3	1:H:219:ILE:HD11	1.81	0.63
1:I:159:THR:O	1:I:161:PRO:HD3	1.99	0.63
1:I:159:THR:HG21	1:I:185:GLN:HE21	1.63	0.62
1:J:17:LEU:HB3	1:J:38:ILE:CD1	2.30	0.62
1:K:42:LYS:HD3	1:K:200:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:HG3	1:A:108:ALA:HB1	1.80	0.62
1:C:26:ASP:O	1:C:30:VAL:HG23	2.00	0.62
1:D:201:VAL:CG1	1:D:204:SER:HB2	2.30	0.61
1:K:23:ASN:ND2	1:K:26:ASP:H	1.97	0.61
1:A:225:LEU:HD22	1:A:225:LEU:H	1.65	0.61
1:F:156:GLY:O	1:F:180:PRO:HD2	2.00	0.61
1:L:26:ASP:O	1:L:30:VAL:HG23	2.00	0.61
1:D:144:ARG:HH12	1:D:166:ARG:HH21	1.45	0.61
1:D:100:PHE:CG	1:D:101:PRO:HD3	2.36	0.61
1:I:216:ALA:O	1:I:220:GLU:HG2	2.01	0.61
1:G:24:ARG:O	1:G:28:LEU:HG	2.01	0.61
1:D:219:ILE:O	1:D:223:LYS:HG3	2.01	0.61
1:C:37:TYR:CE2	1:C:216:ALA:HB2	2.36	0.61
1:G:141:GLU:HG2	1:H:134:PHE:HE2	1.65	0.60
1:I:29:ARG:O	1:I:33:GLU:HG3	2.01	0.60
1:K:178:ILE:HD12	1:K:200:ILE:HD11	1.82	0.60
1:F:131:ALA:HB3	1:F:160:ARG:NH2	2.15	0.60
1:K:188:ASP:HB3	1:K:191:GLU:HB3	1.83	0.60
1:L:42:LYS:HE2	1:L:70:ASP:OD2	2.01	0.60
1:J:220:GLU:HA	1:J:223:LYS:CG	2.32	0.60
1:E:118:ARG:CZ	1:G:118:ARG:HH21	2.14	0.60
1:J:72:LYS:HB3	1:J:98:HIS:CD2	2.37	0.60
1:B:17:LEU:CB	1:B:38:ILE:HD13	2.31	0.59
1:D:139:ALA:HB3	1:D:163:ARG:HH21	1.67	0.59
1:I:182:VAL:HA	1:I:186:GLY:O	2.02	0.59
1:A:72:LYS:HB3	1:A:98:HIS:CD2	2.37	0.59
1:L:128:HIS:CE1	1:L:131:ALA:HB2	2.37	0.59
1:G:92:ALA:O	1:G:118:ARG:HD3	2.02	0.59
1:G:23:ASN:ND2	1:G:26:ASP:OD2	2.35	0.59
1:C:178:ILE:HD12	1:C:200:ILE:HD11	1.84	0.59
1:E:214:ALA:O	1:E:218:ILE:HG13	2.03	0.59
1:G:142:ILE:O	1:G:145:MET:HB3	2.02	0.59
1:M:37:TYR:HB3	1:M:219:ILE:HD11	1.83	0.59
1:E:220:GLU:OE1	1:E:223:LYS:HD2	2.02	0.59
1:J:17:LEU:CB	1:J:38:ILE:HD13	2.32	0.59
1:M:117:GLY:O	1:M:118:ARG:NH1	2.35	0.59
1:D:26:ASP:O	1:D:30:VAL:HG23	2.02	0.58
1:G:132:GLU:HG2	1:G:136:GLN:NE2	2.17	0.58
1:L:127:SER:HA	1:L:160:ARG:HH12	1.67	0.58
1:A:178:ILE:HD12	1:A:200:ILE:HD11	1.83	0.58
1:A:62:ARG:HH11	1:A:62:ARG:HG2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ALA:O	1:H:219:ILE:HG13	2.03	0.58
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.68	0.58
1:I:24:ARG:O	1:I:28:LEU:HD13	2.03	0.58
1:C:156:GLY:O	1:C:180:PRO:HD2	2.04	0.58
1:E:145:MET:O	1:E:149:LEU:HG	2.04	0.58
1:C:210:ASN:ND2	1:C:213:ALA:HB2	2.19	0.58
1:L:118:ARG:HG2	1:L:118:ARG:HH11	1.69	0.58
1:D:34:VAL:HG12	1:D:212:ALA:HA	1.85	0.57
1:K:158:SER:HB2	1:K:179:SER:OG	2.04	0.57
1:F:72:LYS:HB3	1:F:98:HIS:CD2	2.39	0.57
1:L:156:GLY:O	1:L:180:PRO:HD2	2.04	0.57
1:M:156:GLY:O	1:M:180:PRO:HD2	2.03	0.57
1:B:132:GLU:HG2	1:B:136:GLN:NE2	2.20	0.57
1:B:190:GLY:HA2	1:B:225:LEU:HD21	1.85	0.57
1:E:13:ASN:HD22	1:E:219:ILE:HG23	1.69	0.57
1:F:125:GLU:HB3	1:F:157:PRO:HD3	1.85	0.57
1:G:37:TYR:HB3	1:G:219:ILE:HD11	1.84	0.57
1:I:158:SER:HB2	1:I:179:SER:O	2.03	0.57
1:K:37:TYR:HB3	1:K:219:ILE:HD11	1.84	0.57
1:E:152:LYS:NZ	1:E:152:LYS:HB3	2.19	0.57
1:K:21:LEU:O	1:K:47:LEU:HD13	2.04	0.57
1:G:141:GLU:HG2	1:H:134:PHE:CE2	2.39	0.57
1:I:127:SER:HB3	1:I:159:THR:OG1	2.05	0.57
1:K:23:ASN:HD22	1:K:26:ASP:CG	2.07	0.57
1:L:220:GLU:OE1	1:L:223:LYS:HD3	2.05	0.56
1:G:55:ILE:HD11	1:G:59:PHE:HE1	1.69	0.56
1:J:166:ARG:HG3	1:J:166:ARG:HH11	1.68	0.56
1:L:189:PRO:O	1:L:193:LEU:HG	2.06	0.56
1:L:38:ILE:C	1:L:38:ILE:HD12	2.26	0.56
1:A:43:ILE:HD12	1:A:67:ILE:HD12	1.88	0.56
1:B:219:ILE:O	1:B:223:LYS:HG3	2.04	0.56
1:E:193:LEU:HD11	1:E:222:ILE:HD12	1.87	0.56
1:F:29:ARG:HG2	1:F:33:GLU:OE2	2.05	0.56
1:E:118:ARG:NH2	1:G:118:ARG:HE	2.03	0.56
1:H:56:ILE:O	1:H:60:ARG:HG3	2.06	0.56
1:I:158:SER:HB3	1:I:180:PRO:O	2.05	0.56
1:A:203:ARG:NH1	1:B:78:GLU:HG2	2.20	0.56
1:J:120:VAL:O	1:J:153:ASN:HB2	2.05	0.56
1:C:14:ARG:NH2	1:M:209:ASP:OD1	2.38	0.56
1:D:201:VAL:HG13	1:D:204:SER:HB2	1.88	0.56
1:D:56:ILE:HG23	1:D:67:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:LEU:O	1:E:47:LEU:HD13	2.06	0.56
1:A:203:ARG:HH12	1:B:78:GLU:HG2	1.72	0.55
1:B:38:ILE:HD11	1:B:41:VAL:HG22	1.88	0.55
1:L:193:LEU:HD12	1:L:225:LEU:HD12	1.88	0.55
1:J:156:GLY:O	1:J:180:PRO:HD2	2.07	0.55
1:K:38:ILE:HD12	1:K:38:ILE:C	2.26	0.55
1:L:219:ILE:O	1:L:223:LYS:HG3	2.06	0.55
1:E:125:GLU:O	1:E:157:PRO:HD3	2.06	0.55
1:D:12:MET:HG2	1:D:13:ASN:HD22	1.72	0.55
1:L:36:GLU:HG3	1:L:37:TYR:CD1	2.41	0.55
1:C:225:LEU:N	1:C:225:LEU:HD12	2.22	0.55
1:E:61:LYS:HE3	1:G:9:MET:HA	1.87	0.55
1:K:193:LEU:CD2	1:K:199:ILE:HG23	2.37	0.55
1:H:29:ARG:HG2	1:H:33:GLU:OE2	2.07	0.55
1:L:127:SER:HA	1:L:160:ARG:NH1	2.21	0.55
1:D:139:ALA:HB3	1:D:163:ARG:NH2	2.21	0.55
1:K:130:GLY:HA3	1:L:104:ASP:OD1	2.07	0.55
1:D:72:LYS:NZ	2:D:229:H2U:H62	2.22	0.55
1:J:37:TYR:OH	1:J:216:ALA:HB2	2.07	0.55
1:J:56:ILE:O	1:J:60:ARG:HG3	2.07	0.55
1:M:107:ARG:NH2	1:M:149:LEU:CD2	2.69	0.54
1:M:10:ASP:OD2	1:M:11:VAL:C	2.45	0.54
1:A:37:TYR:HB3	1:A:219:ILE:HD11	1.89	0.54
1:C:203:ARG:NH1	1:D:78:GLU:HG2	2.22	0.54
1:K:131:ALA:HB3	1:K:160:ARG:HH22	1.73	0.54
1:J:220:GLU:C	1:J:222:ILE:H	2.09	0.54
1:L:98:HIS:CE1	1:L:123:LEU:HD23	2.43	0.54
1:M:20:ASP:HA	3:M:230:HOH:O	2.06	0.54
1:J:210:ASN:OD1	1:J:213:ALA:HB2	2.07	0.54
1:D:166:ARG:O	1:D:169:GLU:HB3	2.06	0.54
1:H:203:ARG:HB3	1:H:207:LEU:HD12	1.89	0.54
1:G:192:THR:HG21	1:G:199:ILE:HG22	1.89	0.54
1:H:23:ASN:HD21	1:H:26:ASP:CG	2.10	0.54
1:A:64:GLY:HA2	1:J:66:ARG:HE	1.73	0.54
1:C:178:ILE:HG22	1:C:198:ALA:HB3	1.90	0.53
1:L:190:GLY:HA2	1:L:193:LEU:HD12	1.90	0.53
1:D:210:ASN:OD1	1:D:213:ALA:HB2	2.09	0.53
1:F:214:ALA:O	1:F:218:ILE:HG13	2.08	0.53
1:G:132:GLU:HG3	1:G:160:ARG:NH2	2.23	0.53
1:D:193:LEU:HD12	1:D:222:ILE:HD13	1.91	0.53
1:E:166:ARG:O	1:E:169:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:ARG:HG2	1:E:207:LEU:CD1	2.39	0.53
1:G:34:VAL:O	1:G:38:ILE:HG12	2.08	0.53
1:A:17:LEU:HB2	1:A:38:ILE:HD13	1.89	0.53
1:G:29:ARG:HG2	1:G:33:GLU:OE2	2.09	0.53
1:I:203:ARG:HG3	2:I:229:H2U:OP2	2.09	0.53
1:A:29:ARG:HG2	1:A:33:GLU:OE2	2.09	0.53
1:C:38:ILE:HD12	1:C:38:ILE:C	2.29	0.53
1:G:24:ARG:HB2	1:G:51:GLU:CG	2.39	0.53
1:K:151:VAL:HB	1:K:154:TYR:OH	2.08	0.53
1:L:100:PHE:CG	1:L:101:PRO:HD3	2.44	0.53
1:M:9:MET:O	1:M:9:MET:CG	2.56	0.53
1:H:214:ALA:O	1:H:218:ILE:HG13	2.09	0.52
1:K:158:SER:OG	1:K:182:VAL:HG22	2.09	0.52
1:K:10:ASP:HB3	1:K:66:ARG:NH1	2.22	0.52
1:M:152:LYS:HB3	1:M:152:LYS:NZ	2.24	0.52
1:K:23:ASN:ND2	1:K:26:ASP:OD2	2.41	0.52
1:L:38:ILE:O	1:L:38:ILE:HD12	2.09	0.52
1:J:102:GLY:O	1:J:106:VAL:HG23	2.09	0.52
1:I:129:PRO:O	1:I:131:ALA:N	2.43	0.52
1:C:72:LYS:HB3	1:C:98:HIS:CD2	2.45	0.52
1:C:9:MET:HB2	3:C:300:HOH:O	2.08	0.52
1:B:23:ASN:HD21	1:B:25:ASP:HB2	1.75	0.52
1:C:85:ARG:NH1	1:C:115:GLU:OE2	2.43	0.52
1:K:189:PRO:CB	1:K:222:ILE:HD11	2.32	0.52
1:C:15:LEU:HD22	1:C:38:ILE:CG2	2.37	0.52
1:I:163:ARG:HB3	1:I:163:ARG:NH1	2.25	0.52
1:L:162:GLU:OE1	1:L:162:GLU:N	2.43	0.52
1:L:158:SER:HB3	1:L:182:VAL:HG13	1.91	0.52
1:F:37:TYR:CZ	1:F:216:ALA:HB2	2.45	0.52
1:G:59:PHE:CB	1:G:67:ILE:HD11	2.40	0.52
1:J:193:LEU:HD21	1:J:199:ILE:HG23	1.92	0.51
1:A:72:LYS:HE2	1:B:75:ASP:CG	2.30	0.51
1:B:17:LEU:HB3	1:B:38:ILE:HD13	1.91	0.51
1:E:14:ARG:HH21	1:E:193:LEU:HD22	1.75	0.51
1:H:30:VAL:O	1:H:34:VAL:HG22	2.10	0.51
1:L:158:SER:CB	1:L:182:VAL:HG13	2.40	0.51
1:E:37:TYR:HB3	1:E:219:ILE:HD11	1.92	0.51
1:J:189:PRO:HB3	1:J:222:ILE:HD11	1.93	0.51
1:L:96:ILE:HG12	1:L:121:PHE:HB2	1.92	0.51
1:E:124:THR:HG22	1:E:142:ILE:HG22	1.92	0.51
1:I:37:TYR:N	1:I:37:TYR:CD1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HB3	1:B:98:HIS:CD2	2.45	0.51
1:F:21:LEU:HD13	1:F:26:ASP:HB3	1.91	0.51
1:G:206:TYR:CD1	1:G:207:LEU:HG	2.45	0.51
1:G:24:ARG:HB2	1:G:51:GLU:CD	2.31	0.51
1:J:17:LEU:HB2	1:J:38:ILE:HD13	1.91	0.51
1:J:214:ALA:O	1:J:218:ILE:HG13	2.11	0.51
1:C:12:MET:HG2	1:C:13:ASN:ND2	2.25	0.51
1:E:201:VAL:CG1	1:E:204:SER:HB3	2.40	0.51
1:H:23:ASN:HA	1:H:51:GLU:OE2	2.11	0.51
1:I:38:ILE:O	1:I:38:ILE:HD12	2.10	0.51
1:F:193:LEU:HD12	1:F:222:ILE:HG21	1.91	0.51
1:I:121:PHE:HB3	1:I:155:VAL:HG23	1.92	0.51
1:M:166:ARG:O	1:M:169:GLU:HG2	2.10	0.51
1:E:14:ARG:NH2	1:E:193:LEU:HD22	2.26	0.50
1:E:56:ILE:HG23	1:E:67:ILE:HG21	1.94	0.50
1:F:219:ILE:O	1:F:223:LYS:HB2	2.11	0.50
1:F:72:LYS:NZ	2:F:229:H2U:H62	2.27	0.50
1:J:193:LEU:HD11	1:J:222:ILE:HD13	1.93	0.50
1:F:162:GLU:HG2	1:F:163:ARG:N	2.25	0.50
1:L:206:TYR:CE1	1:L:207:LEU:HG	2.46	0.50
1:L:42:LYS:HD3	1:L:200:ILE:HG21	1.93	0.50
1:B:210:ASN:ND2	1:B:213:ALA:CB	2.72	0.50
1:J:222:ILE:O	1:J:222:ILE:HG22	2.11	0.50
1:L:33:GLU:OE1	1:L:211:PRO:HD2	2.11	0.50
1:G:192:THR:CG2	1:G:199:ILE:HG22	2.42	0.50
1:I:183:GLY:O	1:I:184:ALA:HB2	2.11	0.50
1:K:29:ARG:O	1:K:33:GLU:HG3	2.11	0.50
1:M:38:ILE:C	1:M:38:ILE:HD12	2.32	0.50
1:E:34:VAL:HG12	1:E:212:ALA:HA	1.93	0.50
1:H:98:HIS:CE1	1:H:123:LEU:HD23	2.46	0.50
1:J:26:ASP:O	1:J:30:VAL:HG23	2.12	0.50
1:A:225:LEU:N	1:A:225:LEU:HD22	2.26	0.50
1:B:14:ARG:NH2	1:B:196:ALA:O	2.44	0.50
1:L:45:TYR:N	1:L:46:PRO:HD2	2.26	0.50
1:A:5:ARG:CG	1:A:6:VAL:N	2.73	0.50
1:F:205:ILE:HD11	1:F:218:ILE:HD12	1.94	0.50
1:D:38:ILE:HD12	1:D:38:ILE:O	2.12	0.50
1:J:166:ARG:O	1:J:169:GLU:HB3	2.12	0.50
1:L:203:ARG:HA	1:L:206:TYR:CE1	2.46	0.50
1:L:26:ASP:HA	1:L:29:ARG:HH12	1.77	0.50
1:L:30:VAL:HG13	1:L:211:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:SER:HB2	1:I:179:SER:HB3	1.94	0.50
1:K:87:THR:HG21	1:K:95:ILE:HD12	1.93	0.50
1:L:58:GLU:O	1:L:62:ARG:HB2	2.11	0.50
1:D:23:ASN:OD1	3:D:248:HOH:O	2.19	0.49
1:E:165:SER:HB2	1:E:195:PHE:CZ	2.48	0.49
1:F:223:LYS:C	1:F:225:LEU:N	2.65	0.49
1:I:23:ASN:ND2	1:I:26:ASP:OD2	2.44	0.49
1:M:107:ARG:NH2	1:M:149:LEU:HD23	2.28	0.49
1:F:210:ASN:HB3	1:F:213:ALA:HB3	1.94	0.49
1:G:23:ASN:HD22	1:G:26:ASP:CG	2.13	0.49
1:B:193:LEU:HD11	1:B:222:ILE:HD13	1.94	0.49
1:D:193:LEU:HG	1:D:199:ILE:HG23	1.95	0.49
1:D:222:ILE:O	1:D:225:LEU:HD13	2.11	0.49
1:K:128:HIS:NE2	1:L:101:PRO:O	2.42	0.49
1:K:102:GLY:HA3	1:L:130:GLY:O	2.12	0.49
1:K:55:ILE:HD12	1:K:58:GLU:OE1	2.12	0.49
1:G:59:PHE:HB3	1:G:67:ILE:HD11	1.94	0.49
1:K:95:ILE:HG23	1:K:95:ILE:O	2.11	0.49
1:E:66:ARG:HE	1:E:93:ASP:CG	2.16	0.49
1:F:17:LEU:HD21	1:F:19:MET:HE2	1.93	0.49
1:I:36:GLU:HB2	1:I:37:TYR:CD1	2.48	0.49
1:L:182:VAL:HG21	1:L:199:ILE:HB	1.93	0.49
1:G:214:ALA:O	1:G:218:ILE:HG13	2.13	0.49
1:I:163:ARG:HA	1:I:163:ARG:HH11	1.78	0.49
1:I:225:LEU:N	1:I:225:LEU:HD12	2.28	0.49
1:B:42:LYS:HE2	1:B:200:ILE:HG21	1.95	0.49
1:C:14:ARG:HH11	1:C:193:LEU:HD22	1.76	0.49
1:I:184:ALA:HB1	1:I:203:ARG:NE	2.26	0.49
1:I:224:ASP:HB3	1:I:225:LEU:HD12	1.94	0.49
1:I:48:VAL:CG1	1:I:53:MET:SD	3.01	0.49
1:A:192:THR:HG21	1:A:199:ILE:HG22	1.95	0.48
1:G:132:GLU:HG3	1:G:160:ARG:HH21	1.79	0.48
1:I:75:ASP:CG	1:J:72:LYS:HE2	2.33	0.48
1:M:178:ILE:HD12	1:M:200:ILE:HD11	1.95	0.48
1:H:118:ARG:HH12	1:L:91:GLY:HA2	1.77	0.48
1:D:38:ILE:C	1:D:38:ILE:HD12	2.34	0.48
1:F:155:VAL:HA	1:F:178:ILE:O	2.13	0.48
1:G:72:LYS:HE2	1:H:75:ASP:CG	2.34	0.48
1:I:128:HIS:HB3	1:J:76:ILE:HG22	1.96	0.48
1:K:154:TYR:O	1:K:177:LEU:HD12	2.13	0.48
1:L:166:ARG:O	1:L:170:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:178:ILE:HG22	1:L:198:ALA:HB3	1.96	0.48
1:L:189:PRO:HG2	1:L:190:GLY:H	1.78	0.48
1:M:9:MET:HB2	1:M:66:ARG:HH21	1.78	0.48
1:E:58:GLU:O	1:E:62:ARG:HB2	2.14	0.48
1:I:193:LEU:HD11	1:I:222:ILE:HD13	1.95	0.48
1:K:106:VAL:HG21	1:K:145:MET:CE	2.43	0.48
1:A:5:ARG:HG3	1:A:6:VAL:N	2.13	0.48
1:G:166:ARG:NH1	1:G:170:ILE:HG12	2.28	0.48
1:G:130:GLY:HA3	1:H:104:ASP:OD1	2.14	0.48
1:E:225:LEU:HD12	1:E:225:LEU:N	2.28	0.48
1:I:162:GLU:CD	1:I:163:ARG:HG2	2.34	0.48
1:I:158:SER:CA	1:I:179:SER:HB3	2.44	0.48
1:B:166:ARG:NH1	1:B:169:GLU:OE2	2.46	0.47
1:D:45:TYR:N	1:D:46:PRO:CD	2.77	0.47
1:D:58:GLU:O	1:D:62:ARG:HB2	2.13	0.47
1:I:36:GLU:HB2	1:I:37:TYR:CE1	2.48	0.47
1:L:181:GLY:O	1:L:185:GLN:HB2	2.13	0.47
1:B:87:THR:HG21	1:B:95:ILE:HD12	1.96	0.47
1:J:81:GLU:HG2	1:J:85:ARG:HH12	1.79	0.47
1:B:100:PHE:CG	1:B:101:PRO:HD3	2.50	0.47
1:I:34:VAL:C	1:I:36:GLU:H	2.17	0.47
1:L:193:LEU:HD11	1:L:222:ILE:HG12	1.96	0.47
1:G:26:ASP:O	1:G:30:VAL:HG23	2.15	0.47
1:D:205:ILE:HG12	1:D:214:ALA:CB	2.45	0.47
1:J:215:ALA:O	1:J:219:ILE:HG13	2.14	0.47
1:L:139:ALA:HB3	1:L:163:ARG:HH21	1.79	0.47
1:J:17:LEU:CB	1:J:38:ILE:CD1	2.91	0.47
1:B:85:ARG:NH1	1:B:115:GLU:OE1	2.37	0.47
1:C:72:LYS:HE2	1:D:75:ASP:CG	2.34	0.47
1:I:18:ALA:HB2	1:I:200:ILE:CG2	2.45	0.47
1:J:162:GLU:HG2	1:J:163:ARG:N	2.30	0.47
1:J:219:ILE:HG22	1:J:223:LYS:HZ1	1.79	0.47
1:L:182:VAL:HA	1:L:187:GLY:HA3	1.97	0.47
1:D:156:GLY:O	1:D:180:PRO:HD2	2.14	0.47
1:H:182:VAL:HA	1:H:187:GLY:CA	2.44	0.47
1:M:215:ALA:O	1:M:219:ILE:HG13	2.15	0.47
1:M:72:LYS:HB3	1:M:98:HIS:CD2	2.50	0.47
1:A:9:MET:HE2	1:A:66:ARG:HD3	1.97	0.47
1:D:48:VAL:HG11	1:D:53:MET:SD	2.55	0.47
1:F:223:LYS:O	1:F:225:LEU:N	2.45	0.47
1:I:213:ALA:O	1:I:216:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:201:VAL:HG11	1:L:205:ILE:HG13	1.96	0.47
1:E:94:ALA:HB2	1:E:119:GLU:HB2	1.96	0.47
1:H:145:MET:HA	3:H:315:HOH:O	2.14	0.47
1:I:162:GLU:OE2	1:I:163:ARG:HG2	2.14	0.47
1:G:44:GLY:O	1:G:48:VAL:HG13	2.14	0.46
1:I:159:THR:C	1:I:161:PRO:HD3	2.36	0.46
1:J:138:ALA:O	1:J:142:ILE:HG13	2.16	0.46
1:K:125:GLU:O	1:K:157:PRO:HG3	2.15	0.46
1:K:162:GLU:HG2	1:K:163:ARG:N	2.30	0.46
1:K:188:ASP:HB3	1:K:191:GLU:CB	2.45	0.46
1:K:45:TYR:N	1:K:46:PRO:CD	2.77	0.46
1:C:66:ARG:CG	1:C:66:ARG:HH11	2.28	0.46
1:D:15:LEU:HG	1:D:38:ILE:HG21	1.96	0.46
1:D:78:GLU:CD	1:D:78:GLU:H	2.19	0.46
1:I:158:SER:HB2	1:I:179:SER:CB	2.45	0.46
1:C:210:ASN:HB3	3:C:243:HOH:O	2.14	0.46
1:G:162:GLU:HG2	1:G:163:ARG:N	2.29	0.46
1:H:19:MET:HG3	1:H:47:LEU:HD22	1.97	0.46
1:C:224:ASP:C	1:C:225:LEU:HD12	2.36	0.46
1:C:52:GLY:O	1:C:55:ILE:HG22	2.15	0.46
1:K:39:ASP:O	1:K:65:CYS:HB2	2.14	0.46
1:L:28:LEU:HD11	1:L:58:GLU:OE1	2.15	0.46
1:C:78:GLU:H	1:C:78:GLU:CD	2.19	0.46
1:E:138:ALA:HB1	1:F:134:PHE:CD2	2.50	0.46
1:H:36:GLU:HG3	1:H:37:TYR:CD1	2.50	0.46
1:I:138:ALA:C	1:I:140:ASP:N	2.68	0.46
1:J:159:THR:O	1:J:160:ARG:HG2	2.15	0.46
1:L:110:LEU:HD21	1:L:151:VAL:HG22	1.97	0.46
1:D:225:LEU:HD12	1:D:225:LEU:N	2.29	0.46
1:E:13:ASN:HD22	1:E:219:ILE:CG2	2.28	0.46
1:E:178:ILE:HD12	1:E:200:ILE:HD11	1.98	0.46
1:G:22:MET:SD	1:H:82:LYS:HB3	2.56	0.46
1:L:20:ASP:HB2	1:L:206:TYR:OH	2.16	0.46
1:B:89:LYS:O	1:D:117:GLY:HA3	2.15	0.46
1:F:162:GLU:HG2	1:F:163:ARG:HG2	1.96	0.46
1:G:158:SER:OG	1:G:182:VAL:HG22	2.16	0.46
1:L:181:GLY:HA2	1:L:185:GLN:NE2	2.31	0.46
1:F:18:ALA:HB2	1:F:200:ILE:CG2	2.46	0.46
1:G:132:GLU:HG2	1:G:136:GLN:HE22	1.79	0.46
1:J:78:GLU:H	1:J:78:GLU:CD	2.18	0.46
1:D:35:ARG:HD3	1:D:63:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:VAL:HG21	1:E:199:ILE:HB	1.98	0.46
1:G:158:SER:HB3	1:G:180:PRO:O	2.15	0.46
1:J:52:GLY:O	1:J:55:ILE:HG22	2.16	0.46
1:L:182:VAL:HA	1:L:187:GLY:CA	2.45	0.46
1:M:88:PHE:CD1	1:M:118:ARG:HG3	2.51	0.46
1:D:17:LEU:HD21	1:D:19:MET:HE3	1.97	0.46
1:F:37:TYR:CD2	1:F:219:ILE:HD12	2.50	0.46
1:G:165:SER:HA	1:G:195:PHE:CD2	2.51	0.46
1:L:224:ASP:O	1:L:225:LEU:HD23	2.16	0.46
1:F:78:GLU:H	1:F:78:GLU:CD	2.19	0.45
1:G:78:GLU:CD	1:G:78:GLU:H	2.20	0.45
1:H:24:ARG:NH1	1:H:24:ARG:HG2	2.31	0.45
1:I:193:LEU:CD1	1:I:222:ILE:HD13	2.46	0.45
1:K:188:ASP:OD2	1:K:191:GLU:HB2	2.16	0.45
1:B:181:GLY:HA2	1:B:185:GLN:NE2	2.31	0.45
1:B:222:ILE:O	1:B:222:ILE:HG22	2.15	0.45
1:D:213:ALA:O	1:D:216:ALA:HB3	2.16	0.45
1:I:101:PRO:O	1:J:128:HIS:NE2	2.50	0.45
1:A:143:ALA:O	1:A:147:VAL:HG23	2.16	0.45
1:C:85:ARG:HH12	1:C:115:GLU:CD	2.15	0.45
1:D:12:MET:HG2	1:D:13:ASN:ND2	2.31	0.45
1:E:59:PHE:O	1:E:63:PHE:HD1	1.98	0.45
1:H:138:ALA:O	1:H:142:ILE:HG13	2.17	0.45
1:L:30:VAL:HG11	1:L:206:TYR:CB	2.46	0.45
1:F:222:ILE:HD12	1:F:222:ILE:C	2.37	0.45
1:F:9:MET:O	1:F:9:MET:HG3	2.16	0.45
1:J:17:LEU:HB3	1:J:38:ILE:HD13	1.98	0.45
1:K:78:GLU:CD	1:K:78:GLU:H	2.19	0.45
1:L:152:LYS:HB3	1:L:152:LYS:HZ2	1.80	0.45
1:A:58:GLU:O	1:A:62:ARG:HB2	2.17	0.45
1:B:210:ASN:HD22	1:B:213:ALA:CB	2.29	0.45
1:C:158:SER:OG	1:C:187:GLY:HA3	2.16	0.45
1:C:78:GLU:HG2	1:D:203:ARG:NH1	2.31	0.45
1:G:85:ARG:HG3	1:G:85:ARG:HH11	1.82	0.45
1:L:132:GLU:HG2	1:L:136:GLN:OE1	2.17	0.45
1:B:17:LEU:HB3	1:B:38:ILE:CD1	2.46	0.45
1:C:123:LEU:HA	1:C:155:VAL:HB	1.99	0.45
1:G:9:MET:HE2	1:G:66:ARG:NH1	2.32	0.45
1:I:180:PRO:HB3	1:I:200:ILE:CD1	2.46	0.45
1:L:107:ARG:HG3	1:L:111:ASN:HD21	1.81	0.45
1:B:223:LYS:C	1:B:225:LEU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:VAL:C	1:I:36:GLU:N	2.70	0.45
1:C:220:GLU:OE1	1:C:220:GLU:HA	2.17	0.45
1:D:17:LEU:HD21	1:D:19:MET:CE	2.47	0.45
1:D:58:GLU:HG2	1:D:62:ARG:HD2	1.99	0.45
1:E:14:ARG:NE	1:E:193:LEU:HD22	2.32	0.45
1:G:201:VAL:CG1	1:G:204:SER:HB2	2.47	0.45
1:I:78:GLU:CD	1:I:78:GLU:H	2.21	0.45
1:A:130:GLY:HA3	1:B:104:ASP:OD1	2.16	0.44
1:D:72:LYS:HB3	1:D:98:HIS:CD2	2.53	0.44
1:E:118:ARG:HH12	1:G:91:GLY:HA2	1.81	0.44
1:D:224:ASP:C	1:D:225:LEU:HD12	2.37	0.44
1:E:14:ARG:HE	1:E:193:LEU:HD22	1.82	0.44
1:F:17:LEU:HD21	1:F:19:MET:CE	2.47	0.44
1:G:24:ARG:HG2	1:G:24:ARG:HH11	1.82	0.44
1:C:14:ARG:NH1	1:C:197:ASP:O	2.51	0.44
1:E:45:TYR:N	1:E:46:PRO:CD	2.80	0.44
1:H:24:ARG:HH11	1:H:24:ARG:HG2	1.82	0.44
1:J:163:ARG:HA	1:J:163:ARG:NH1	2.25	0.44
1:J:17:LEU:HB3	1:J:38:ILE:HD11	1.99	0.44
1:K:215:ALA:O	1:K:219:ILE:HG13	2.18	0.44
1:L:26:ASP:HA	1:L:29:ARG:NH1	2.33	0.44
1:M:72:LYS:NZ	2:M:229:H2U:H62	2.32	0.44
1:E:72:LYS:HE2	1:F:75:ASP:CG	2.37	0.44
1:G:18:ALA:HA	1:G:42:LYS:HB3	2.00	0.44
1:G:33:GLU:O	1:G:212:ALA:HB2	2.17	0.44
1:J:157:PRO:O	1:J:164:LEU:HD13	2.17	0.44
1:L:125:GLU:HB2	1:L:139:ALA:HB1	1.98	0.44
1:B:78:GLU:H	1:B:78:GLU:CD	2.21	0.44
1:C:78:GLU:HG2	1:D:203:ARG:HH12	1.83	0.44
1:J:166:ARG:HG3	1:J:166:ARG:NH1	2.32	0.44
1:K:125:GLU:HA	1:K:135:ILE:CG2	2.48	0.44
1:F:128:HIS:O	1:F:131:ALA:HB3	2.18	0.44
1:F:88:PHE:CD1	1:F:118:ARG:HG3	2.53	0.44
1:K:219:ILE:O	1:K:223:LYS:HG3	2.17	0.44
1:L:78:GLU:H	1:L:78:GLU:CD	2.20	0.44
1:C:66:ARG:NH1	1:C:93:ASP:HB3	2.33	0.44
1:E:75:ASP:CG	1:F:72:LYS:HE2	2.38	0.44
1:G:45:TYR:N	1:G:46:PRO:CD	2.80	0.44
1:K:128:HIS:HB3	1:L:76:ILE:HG22	1.99	0.44
1:B:222:ILE:O	1:B:225:LEU:HB2	2.16	0.44
1:B:17:LEU:HB2	1:B:38:ILE:HD13	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ILE:HG12	1:D:214:ALA:HB3	2.00	0.44
1:D:219:ILE:HG22	1:D:223:LYS:HG3	2.00	0.44
1:E:9:MET:CB	3:E:249:HOH:O	2.60	0.44
1:F:139:ALA:HB3	1:F:163:ARG:HH22	1.83	0.44
1:G:94:ALA:HB2	1:G:119:GLU:HB2	2.00	0.44
1:H:19:MET:HG3	1:H:47:LEU:CD2	2.48	0.44
1:I:138:ALA:C	1:I:140:ASP:H	2.21	0.44
1:M:107:ARG:HH21	1:M:149:LEU:CD2	2.30	0.44
1:D:203:ARG:C	1:D:205:ILE:H	2.21	0.44
1:J:34:VAL:HG12	1:J:212:ALA:HA	1.98	0.44
1:A:166:ARG:NH1	1:A:169:GLU:HG3	2.33	0.43
1:B:38:ILE:O	1:B:38:ILE:HG13	2.15	0.43
1:C:81:GLU:HG3	1:C:108:ALA:HB1	2.00	0.43
1:E:78:GLU:H	1:E:78:GLU:CD	2.21	0.43
1:G:206:TYR:CE1	1:G:207:LEU:HG	2.53	0.43
1:I:180:PRO:CA	1:I:200:ILE:HB	2.47	0.43
1:K:222:ILE:HG22	1:K:222:ILE:O	2.18	0.43
1:L:193:LEU:CD1	1:L:222:ILE:HG23	2.48	0.43
1:L:183:GLY:HA3	1:L:204:SER:OG	2.18	0.43
1:K:60:ARG:O	1:K:64:GLY:N	2.47	0.43
1:K:78:GLU:HG2	1:L:203:ARG:HH12	1.83	0.43
1:B:125:GLU:HG2	1:B:157:PRO:HG3	2.00	0.43
1:C:14:ARG:NH1	1:C:193:LEU:HD22	2.33	0.43
1:D:72:LYS:CE	2:D:229:H2U:H62	2.48	0.43
1:G:166:ARG:HH12	1:G:170:ILE:HG12	1.83	0.43
1:G:156:GLY:O	1:G:180:PRO:HD2	2.18	0.43
1:H:35:ARG:HH12	1:H:39:ASP:HA	1.80	0.43
1:I:192:THR:C	1:I:194:ARG:H	2.21	0.43
1:K:138:ALA:O	1:K:142:ILE:HG13	2.18	0.43
1:K:166:ARG:HG3	1:K:170:ILE:HD11	2.00	0.43
1:C:220:GLU:HA	1:C:223:LYS:HB2	2.00	0.43
1:H:21:LEU:HD12	1:H:27:ALA:HA	2.01	0.43
1:K:225:LEU:N	1:K:225:LEU:HD12	2.33	0.43
1:L:72:LYS:HB3	1:L:98:HIS:CD2	2.54	0.43
1:D:66:ARG:HG2	1:D:93:ASP:CB	2.48	0.43
1:E:139:ALA:O	1:E:142:ILE:HB	2.17	0.43
1:F:182:VAL:HG11	1:F:189:PRO:HG3	2.00	0.43
1:F:178:ILE:HA	1:F:198:ALA:O	2.19	0.43
1:H:23:ASN:OD1	1:H:26:ASP:OD1	2.36	0.43
1:G:75:ASP:CG	1:H:72:LYS:HE2	2.38	0.43
1:J:152:LYS:HE2	1:J:152:LYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:VAL:HG21	1:K:145:MET:HE3	1.99	0.43
1:L:42:LYS:HD2	1:L:200:ILE:HD13	1.99	0.43
1:L:206:TYR:CD1	1:L:207:LEU:HG	2.53	0.43
1:H:34:VAL:HG12	1:H:212:ALA:HA	1.99	0.43
1:I:219:ILE:O	1:I:223:LYS:N	2.51	0.43
1:J:81:GLU:CG	1:J:85:ARG:HH12	2.31	0.43
1:L:40:THR:HG23	1:L:66:ARG:HB2	2.00	0.43
1:M:72:LYS:CE	2:M:229:H2U:H62	2.48	0.43
1:B:132:GLU:HG2	1:B:136:GLN:HE21	1.83	0.43
1:E:57:ALA:O	1:E:61:LYS:HD3	2.18	0.43
1:G:219:ILE:O	1:G:223:LYS:HG3	2.18	0.43
1:I:182:VAL:HG13	1:I:187:GLY:O	2.19	0.43
1:L:100:PHE:N	1:L:101:PRO:CD	2.82	0.43
1:E:201:VAL:HG13	1:E:204:SER:HB3	2.01	0.43
1:F:206:TYR:CD1	1:F:207:LEU:HG	2.54	0.43
1:G:182:VAL:HG21	1:G:199:ILE:HB	2.01	0.43
1:H:78:GLU:CD	1:H:78:GLU:H	2.22	0.43
1:I:126:MET:HA	2:I:229:H2U:O4	2.19	0.43
1:I:81:GLU:HG3	1:I:108:ALA:HB1	2.00	0.43
1:D:193:LEU:HG	1:D:199:ILE:CG2	2.48	0.43
1:E:13:ASN:ND2	1:E:219:ILE:HD13	2.34	0.43
1:H:162:GLU:HG2	1:H:163:ARG:N	2.33	0.43
1:C:45:TYR:N	1:C:46:PRO:CD	2.82	0.42
1:F:206:TYR:CD1	1:F:206:TYR:C	2.92	0.42
1:F:30:VAL:O	1:F:34:VAL:HG22	2.18	0.42
1:H:102:GLY:O	1:H:106:VAL:HG23	2.19	0.42
1:I:217:GLY:O	1:I:220:GLU:HB2	2.19	0.42
1:L:29:ARG:HG2	1:L:33:GLU:OE2	2.19	0.42
1:G:181:GLY:HA2	1:G:185:GLN:HB2	2.01	0.42
1:M:220:GLU:C	1:M:222:ILE:H	2.23	0.42
1:B:52:GLY:O	1:B:55:ILE:HG22	2.18	0.42
1:G:184:ALA:HB1	1:G:203:ARG:HE	1.85	0.42
1:I:26:ASP:OD1	1:I:29:ARG:NH1	2.52	0.42
1:J:220:GLU:OE1	1:J:223:LYS:HD2	2.19	0.42
1:A:75:ASP:CG	1:B:72:LYS:HE2	2.40	0.42
1:A:78:GLU:CD	1:A:78:GLU:H	2.22	0.42
1:A:87:THR:HG21	1:A:95:ILE:HD12	2.02	0.42
1:B:156:GLY:O	1:B:180:PRO:HD2	2.20	0.42
1:B:30:VAL:HG13	1:B:211:PRO:HG2	2.01	0.42
1:B:37:TYR:HB3	1:B:219:ILE:HD11	2.02	0.42
1:B:97:VAL:HG21	1:B:109:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:ALA:HB2	1:H:120:VAL:HG23	2.01	0.42
1:C:158:SER:HB3	1:C:180:PRO:O	2.20	0.42
1:L:118:ARG:CG	1:L:118:ARG:HH11	2.31	0.42
1:B:38:ILE:HD12	1:B:40:THR:O	2.19	0.42
1:G:138:ALA:O	1:G:142:ILE:HG13	2.19	0.42
1:H:36:GLU:HG3	1:H:37:TYR:CE1	2.53	0.42
1:K:202:GLY:O	1:K:204:SER:N	2.53	0.42
1:L:88:PHE:CD1	1:L:118:ARG:HG3	2.54	0.42
1:M:54:ASP:HA	3:M:240:HOH:O	2.20	0.42
1:B:152:LYS:HB3	1:B:152:LYS:NZ	2.35	0.42
1:C:85:ARG:NH1	1:C:115:GLU:CD	2.73	0.42
1:C:30:VAL:O	1:C:34:VAL:HG22	2.19	0.42
1:G:155:VAL:HA	1:G:178:ILE:O	2.19	0.42
1:I:203:ARG:HG2	1:I:206:TYR:OH	2.20	0.42
1:M:11:VAL:CG1	3:M:234:HOH:O	2.67	0.42
1:M:72:LYS:O	1:M:73:VAL:C	2.58	0.42
1:C:134:PHE:HE2	1:D:141:GLU:HB3	1.84	0.42
1:D:158:SER:HB2	1:D:192:THR:OG1	2.20	0.42
1:H:45:TYR:O	1:H:49:LEU:HB2	2.19	0.42
1:M:78:GLU:CD	1:M:78:GLU:H	2.22	0.42
1:C:130:GLY:HA3	1:D:104:ASP:OD1	2.20	0.42
1:D:188:ASP:HA	1:D:189:PRO:HD3	1.92	0.42
1:E:49:LEU:HB3	1:F:53:MET:HE2	2.01	0.42
1:I:208:ALA:C	1:I:210:ASN:H	2.22	0.42
1:L:12:MET:N	1:L:39:ASP:OD1	2.49	0.42
1:M:45:TYR:N	1:M:46:PRO:CD	2.82	0.42
1:A:210:ASN:ND2	1:A:213:ALA:HB2	2.34	0.42
1:E:52:GLY:O	1:E:55:ILE:HG22	2.19	0.42
1:G:12:MET:O	1:G:13:ASN:HB2	2.20	0.42
1:G:126:MET:HA	2:G:229:H2U:O4	2.20	0.42
1:I:42:LYS:NZ	3:I:303:HOH:O	2.52	0.42
1:L:201:VAL:CG1	1:L:205:ILE:HG13	2.50	0.42
1:L:30:VAL:HG11	1:L:206:TYR:HB3	2.02	0.42
1:B:166:ARG:HA	1:B:169:GLU:HG2	2.02	0.41
1:C:100:PHE:HB3	1:C:101:PRO:HD3	2.02	0.41
1:D:193:LEU:CD2	1:D:199:ILE:HG23	2.49	0.41
1:F:182:VAL:CG1	1:F:189:PRO:HG3	2.50	0.41
1:K:152:LYS:NZ	1:K:152:LYS:CB	2.83	0.41
1:M:214:ALA:O	1:M:218:ILE:HG13	2.20	0.41
1:A:225:LEU:CD2	1:A:225:LEU:H	2.32	0.41
1:M:100:PHE:HB3	1:M:101:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HG2	1:B:203:ARG:NH1	2.35	0.41
1:B:100:PHE:N	1:B:101:PRO:CD	2.82	0.41
1:B:33:GLU:OE1	1:B:211:PRO:HD2	2.20	0.41
1:I:96:ILE:HD13	1:I:155:VAL:HG21	2.02	0.41
1:J:193:LEU:CD2	1:J:199:ILE:HG23	2.50	0.41
1:M:118:ARG:HD3	1:M:118:ARG:HH11	1.77	0.41
1:D:14:ARG:HH21	1:D:193:LEU:HD22	1.86	0.41
1:E:156:GLY:O	1:E:180:PRO:HD2	2.21	0.41
1:L:34:VAL:HG12	1:L:212:ALA:HA	2.02	0.41
1:M:10:ASP:OD2	1:M:10:ASP:C	2.57	0.41
1:B:58:GLU:O	1:B:62:ARG:HB2	2.20	0.41
1:E:124:THR:OG1	1:E:167:LEU:HD13	2.19	0.41
1:F:206:TYR:CE1	1:F:207:LEU:HG	2.55	0.41
1:G:88:PHE:O	1:G:91:GLY:N	2.42	0.41
1:H:104:ASP:N	1:H:104:ASP:OD1	2.54	0.41
1:K:162:GLU:OE1	1:K:163:ARG:HG2	2.20	0.41
1:K:72:LYS:HE2	1:L:75:ASP:CG	2.40	0.41
1:K:87:THR:O	1:K:90:ALA:HB3	2.19	0.41
1:M:11:VAL:HG21	1:M:16:ILE:HD11	2.02	0.41
1:C:72:LYS:NZ	2:C:229:H2U:H62	2.35	0.41
1:I:166:ARG:O	1:I:170:ILE:HG13	2.21	0.41
1:I:216:ALA:O	1:I:219:ILE:HG12	2.21	0.41
1:I:30:VAL:HG11	1:I:206:TYR:HA	2.02	0.41
1:K:26:ASP:O	1:K:30:VAL:HG23	2.20	0.41
1:K:24:ARG:HB2	1:K:51:GLU:OE1	2.21	0.41
1:D:193:LEU:HD21	1:D:199:ILE:HG23	2.02	0.41
1:M:125:GLU:HB3	1:M:157:PRO:HD3	2.03	0.41
1:M:73:VAL:HG12	1:M:80:ASN:OD1	2.20	0.41
1:F:26:ASP:O	1:F:30:VAL:HG23	2.20	0.41
1:G:223:LYS:C	1:G:225:LEU:H	2.24	0.41
1:L:29:ARG:O	1:L:33:GLU:HG3	2.20	0.41
1:A:5:ARG:HB3	1:A:7:ASP:OD1	2.21	0.41
1:F:42:LYS:CG	1:F:70:ASP:HB2	2.51	0.41
1:G:81:GLU:HG3	1:G:108:ALA:HB1	2.02	0.41
1:I:34:VAL:HG11	1:I:205:ILE:CG2	2.51	0.41
1:I:35:ARG:NE	1:I:63:PHE:O	2.53	0.41
1:K:113:ALA:HB1	1:K:118:ARG:O	2.20	0.41
1:C:37:TYR:HD2	1:C:219:ILE:HD12	1.86	0.41
1:C:118:ARG:NH1	1:F:118:ARG:NH2	2.69	0.41
1:F:193:LEU:HD21	1:F:199:ILE:HG12	2.02	0.41
1:K:48:VAL:O	1:K:52:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:GLU:CG	1:K:163:ARG:N	2.84	0.41
1:K:37:TYR:CZ	1:K:216:ALA:HB2	2.55	0.41
1:L:99:GLY:CA	1:L:122:LEU:HD11	2.51	0.41
1:A:81:GLU:HG2	1:A:108:ALA:O	2.21	0.40
1:F:15:LEU:HD11	1:F:201:VAL:HG23	2.02	0.40
1:G:160:ARG:O	1:G:163:ARG:HB2	2.21	0.40
1:K:33:GLU:OE1	1:K:211:PRO:HG2	2.21	0.40
1:L:125:GLU:HB2	1:L:139:ALA:CB	2.50	0.40
1:L:78:GLU:O	1:L:81:GLU:HB2	2.20	0.40
1:C:104:ASP:N	1:C:104:ASP:OD1	2.51	0.40
1:D:193:LEU:CD1	1:D:222:ILE:HD13	2.52	0.40
1:G:45:TYR:O	1:G:46:PRO:C	2.59	0.40
1:G:59:PHE:HB2	1:G:67:ILE:HD11	2.03	0.40
1:H:223:LYS:C	1:H:225:LEU:H	2.25	0.40
1:J:201:VAL:HG11	1:J:218:ILE:CD1	2.51	0.40
1:J:21:LEU:HD23	1:J:21:LEU:HA	1.92	0.40
1:K:220:GLU:C	1:K:222:ILE:H	2.25	0.40
1:M:21:LEU:HD23	1:M:21:LEU:HA	1.93	0.40
1:F:128:HIS:O	1:F:131:ALA:CB	2.70	0.40
1:H:35:ARG:NH1	1:H:65:CYS:HB3	2.37	0.40
1:H:87:THR:HG21	1:H:95:ILE:HD12	2.03	0.40
1:K:104:ASP:N	1:K:104:ASP:OD1	2.55	0.40
1:H:125:GLU:O	1:H:157:PRO:HD3	2.21	0.40
1:H:188:ASP:HB3	1:H:191:GLU:HB2	2.03	0.40
1:J:9:MET:HB2	3:J:236:HOH:O	2.20	0.40
1:K:107:ARG:O	1:K:111:ASN:OD1	2.39	0.40
1:K:154:TYR:O	1:K:177:LEU:HA	2.22	0.40
1:K:193:LEU:HD21	1:K:199:ILE:HG23	2.04	0.40
1:M:224:ASP:C	1:M:225:LEU:HD12	2.41	0.40
1:A:45:TYR:O	1:A:46:PRO:C	2.58	0.40
1:A:73:VAL:HG12	1:A:80:ASN:OD1	2.22	0.40
1:E:13:ASN:ND2	1:E:219:ILE:CG2	2.85	0.40
1:F:37:TYR:HD2	1:F:219:ILE:HD12	1.86	0.40
1:I:38:ILE:C	1:I:38:ILE:HD12	2.41	0.40
1:J:12:MET:O	1:J:13:ASN:HB2	2.22	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:K:118:ARG:NH1	1:K:118:ARG:NH1[2_354]	2.08	0.12

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	219/228 (96%)	214 (98%)	5 (2%)	0	100	100
1	B	214/228 (94%)	202 (94%)	12 (6%)	0	100	100
1	C	216/228 (95%)	206 (95%)	10 (5%)	0	100	100
1	D	213/228 (93%)	201 (94%)	10 (5%)	2 (1%)	20	23
1	E	215/228 (94%)	198 (92%)	17 (8%)	0	100	100
1	F	215/228 (94%)	195 (91%)	16 (7%)	4 (2%)	9	8
1	G	215/228 (94%)	198 (92%)	17 (8%)	0	100	100
1	H	214/228 (94%)	200 (94%)	12 (6%)	2 (1%)	20	23
1	I	210/228 (92%)	183 (87%)	22 (10%)	5 (2%)	7	5
1	J	216/228 (95%)	196 (91%)	18 (8%)	2 (1%)	20	23
1	K	214/228 (94%)	191 (89%)	19 (9%)	4 (2%)	9	8
1	L	214/228 (94%)	194 (91%)	18 (8%)	2 (1%)	20	23
1	M	215/228 (94%)	205 (95%)	10 (5%)	0	100	100
All	All	2790/2964 (94%)	2583 (93%)	186 (7%)	21 (1%)	22	26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	184	ALA
1	F	14	ARG
1	I	130	GLY
1	K	203	ARG
1	F	39	ASP
1	F	224	ASP
1	H	189	PRO
1	I	129	PRO
1	J	189	PRO
1	K	130	GLY

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Mol	Chain	Res	Type
1	L	212	ALA
1	F	13	ASN
1	J	222	ILE
1	K	139	ALA
1	D	189	PRO
1	H	223	LYS
1	I	187	GLY
1	D	205	ILE
1	I	193	LEU
1	K	54	ASP
1	L	189	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	175/182 (96%)	173 (99%)	2 (1%)	78	89
1	B	170/182 (93%)	164 (96%)	6 (4%)	41	56
1	C	172/182 (94%)	169 (98%)	3 (2%)	66	81
1	D	169/182 (93%)	168 (99%)	1 (1%)	89	95
1	E	171/182 (94%)	169 (99%)	2 (1%)	75	87
1	F	171/182 (94%)	169 (99%)	2 (1%)	75	87
1	G	171/182 (94%)	167 (98%)	4 (2%)	56	73
1	H	170/182 (93%)	169 (99%)	1 (1%)	89	95
1	I	166/182 (91%)	159 (96%)	7 (4%)	34	47
1	J	172/182 (94%)	169 (98%)	3 (2%)	66	81
1	K	170/182 (93%)	167 (98%)	3 (2%)	64	79
1	L	170/182 (93%)	165 (97%)	5 (3%)	48	64
1	M	171/182 (94%)	169 (99%)	2 (1%)	75	87
All	All	2218/2366 (94%)	2177 (98%)	41 (2%)	64	79

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	157	PRO
1	B	38	ILE
1	B	59	PHE
1	B	62	ARG
1	B	66	ARG
1	B	136	GLN
1	B	167	LEU
1	C	66	ARG
1	C	158	SER
1	C	167	LEU
1	D	195	PHE
1	E	98	HIS
1	E	174	ASP
1	F	81	GLU
1	F	206	TYR
1	G	48	VAL
1	G	140	ASP
1	G	167	LEU
1	G	206	TYR
1	H	210	ASN
1	I	37	TYR
1	I	63	PHE
1	I	132	GLU
1	I	140	ASP
1	I	162	GLU
1	I	166	ARG
1	I	174	ASP
1	J	66	ARG
1	J	210	ASN
1	J	223	LYS
1	K	59	PHE
1	K	140	ASP
1	K	152	LYS
1	L	23	ASN
1	L	66	ARG
1	L	162	GLU
1	L	195	PHE
1	L	206	TYR
1	M	10	ASP
1	M	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	ASN
1	B	136	GLN
1	B	210	ASN
1	C	210	ASN
1	D	13	ASN
1	D	23	ASN
1	D	173	GLN
1	D	210	ASN
1	E	13	ASN
1	E	185	GLN
1	F	13	ASN
1	G	23	ASN
1	G	136	GLN
1	H	210	ASN
1	I	23	ASN
1	I	185	GLN
1	J	210	ASN
1	K	23	ASN
1	K	185	GLN
1	L	98	HIS
1	L	111	ASN
1	M	98	HIS
1	M	210	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 ⓘ

13 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	H2U	A	229	-	21,22,22	1.77	5 (23%)	28,33,33	1.89	5 (17%)
2	H2U	B	229	-	21,22,22	1.61	4 (19%)	28,33,33	1.91	5 (17%)
2	H2U	C	229	-	21,22,22	1.62	6 (28%)	28,33,33	1.93	5 (17%)
2	H2U	D	229	-	21,22,22	1.67	5 (23%)	28,33,33	1.93	5 (17%)
2	H2U	E	229	-	21,22,22	1.61	5 (23%)	28,33,33	1.92	5 (17%)
2	H2U	F	229	-	21,22,22	1.68	6 (28%)	28,33,33	1.93	5 (17%)
2	H2U	G	229	-	21,22,22	1.60	4 (19%)	28,33,33	1.91	5 (17%)
2	H2U	H	229	-	21,22,22	1.66	5 (23%)	28,33,33	1.94	5 (17%)
2	H2U	I	229	-	21,22,22	1.69	5 (23%)	28,33,33	1.95	5 (17%)
2	H2U	J	229	-	21,22,22	1.72	5 (23%)	28,33,33	1.94	5 (17%)
2	H2U	K	229	-	21,22,22	1.70	5 (23%)	28,33,33	1.94	5 (17%)
2	H2U	L	229	-	21,22,22	1.67	5 (23%)	28,33,33	1.95	5 (17%)
2	H2U	M	229	-	21,22,22	1.70	5 (23%)	28,33,33	1.94	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H2U	A	229	-	-	0/10/39/39	0/2/2/2
2	H2U	B	229	-	-	0/10/39/39	0/2/2/2
2	H2U	C	229	-	-	0/10/39/39	0/2/2/2
2	H2U	D	229	-	-	0/10/39/39	0/2/2/2
2	H2U	E	229	-	-	0/10/39/39	0/2/2/2
2	H2U	F	229	-	-	0/10/39/39	0/2/2/2
2	H2U	G	229	-	-	0/10/39/39	0/2/2/2
2	H2U	H	229	-	-	0/10/39/39	0/2/2/2
2	H2U	I	229	-	-	0/10/39/39	0/2/2/2
2	H2U	J	229	-	-	0/10/39/39	0/2/2/2
2	H2U	K	229	-	-	0/10/39/39	0/2/2/2
2	H2U	L	229	-	-	0/10/39/39	0/2/2/2
2	H2U	M	229	-	-	0/10/39/39	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	229	H2U	C2'-C3'	-2.25	1.47	1.53
2	D	229	H2U	C6-N1	2.00	1.49	1.47
2	F	229	H2U	C6-C5	2.01	1.56	1.52
2	H	229	H2U	C6-N1	2.10	1.49	1.47
2	E	229	H2U	C6-N1	2.11	1.49	1.47
2	M	229	H2U	C6-N1	2.21	1.49	1.47
2	F	229	H2U	C6-N1	2.22	1.49	1.47
2	L	229	H2U	C6-N1	2.26	1.49	1.47
2	A	229	H2U	P-OP2	2.31	1.64	1.54
2	I	229	H2U	C6-N1	2.37	1.50	1.47
2	J	229	H2U	C6-N1	2.52	1.50	1.47
2	M	229	H2U	P-OP2	2.54	1.65	1.54
2	K	229	H2U	C6-N1	2.55	1.50	1.47
2	H	229	H2U	P-OP2	2.55	1.65	1.54
2	J	229	H2U	P-OP2	2.55	1.65	1.54
2	F	229	H2U	P-OP2	2.60	1.65	1.54
2	C	229	H2U	C2-N1	2.60	1.39	1.35
2	A	229	H2U	O4'-C1'	2.60	1.48	1.42
2	G	229	H2U	P-OP2	2.61	1.65	1.54
2	D	229	H2U	P-OP2	2.62	1.65	1.54
2	C	229	H2U	P-OP2	2.64	1.65	1.54
2	K	229	H2U	P-OP2	2.65	1.65	1.54
2	C	229	H2U	O4'-C4'	2.66	1.51	1.45
2	E	229	H2U	P-OP2	2.69	1.65	1.54
2	I	229	H2U	P-OP2	2.75	1.66	1.54
2	L	229	H2U	P-OP2	2.78	1.66	1.54
2	G	229	H2U	O4'-C4'	2.78	1.51	1.45
2	C	229	H2U	C6-N1	2.83	1.50	1.47
2	J	229	H2U	O4'-C4'	2.83	1.51	1.45
2	C	229	H2U	O4'-C1'	2.83	1.48	1.42
2	G	229	H2U	O4'-C1'	2.83	1.48	1.42
2	B	229	H2U	O4'-C4'	2.85	1.51	1.45
2	B	229	H2U	P-OP2	2.85	1.66	1.54
2	D	229	H2U	O4'-C1'	2.86	1.49	1.42
2	E	229	H2U	O4'-C4'	2.90	1.51	1.45
2	F	229	H2U	O4'-C4'	2.92	1.51	1.45
2	E	229	H2U	O4'-C1'	2.92	1.49	1.42
2	L	229	H2U	O4'-C1'	2.92	1.49	1.42
2	J	229	H2U	O4'-C1'	2.95	1.49	1.42
2	K	229	H2U	O4'-C4'	2.96	1.51	1.45
2	I	229	H2U	O4'-C4'	2.97	1.51	1.45
2	L	229	H2U	O4'-C4'	2.97	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	229	H2U	O4'-C1'	2.97	1.49	1.42
2	H	229	H2U	O4'-C4'	2.98	1.51	1.45
2	I	229	H2U	O4'-C1'	2.98	1.49	1.42
2	A	229	H2U	C6-N1	2.99	1.50	1.47
2	B	229	H2U	O4'-C1'	3.00	1.49	1.42
2	M	229	H2U	O4'-C1'	3.01	1.49	1.42
2	B	229	H2U	C2-N1	3.02	1.40	1.35
2	E	229	H2U	C2-N1	3.02	1.40	1.35
2	F	229	H2U	O4'-C1'	3.03	1.49	1.42
2	D	229	H2U	O4'-C4'	3.09	1.52	1.45
2	K	229	H2U	O4'-C1'	3.10	1.49	1.42
2	G	229	H2U	C2-N1	3.22	1.40	1.35
2	M	229	H2U	O4'-C4'	3.30	1.52	1.45
2	M	229	H2U	C2-N1	3.38	1.40	1.35
2	H	229	H2U	C2-N1	3.39	1.40	1.35
2	L	229	H2U	C2-N1	3.45	1.40	1.35
2	I	229	H2U	C2-N1	3.47	1.40	1.35
2	A	229	H2U	O4'-C4'	3.47	1.52	1.45
2	F	229	H2U	C2-N1	3.56	1.40	1.35
2	K	229	H2U	C2-N1	3.56	1.40	1.35
2	D	229	H2U	C2-N1	3.63	1.41	1.35
2	J	229	H2U	C2-N1	3.68	1.41	1.35
2	A	229	H2U	C2-N1	3.78	1.41	1.35

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	229	H2U	C4-N3-C2	-5.79	120.85	125.81
2	C	229	H2U	C4-N3-C2	-5.78	120.86	125.81
2	L	229	H2U	C4-N3-C2	-5.76	120.88	125.81
2	J	229	H2U	C4-N3-C2	-5.76	120.88	125.81
2	K	229	H2U	C4-N3-C2	-5.74	120.89	125.81
2	H	229	H2U	C4-N3-C2	-5.71	120.92	125.81
2	M	229	H2U	C4-N3-C2	-5.71	120.92	125.81
2	F	229	H2U	C4-N3-C2	-5.68	120.94	125.81
2	D	229	H2U	C4-N3-C2	-5.64	120.98	125.81
2	E	229	H2U	C4-N3-C2	-5.63	120.99	125.81
2	B	229	H2U	C4-N3-C2	-5.59	121.02	125.81
2	G	229	H2U	C4-N3-C2	-5.54	121.06	125.81
2	A	229	H2U	C4-N3-C2	-5.46	121.13	125.81
2	G	229	H2U	P-O5'-C5'	-4.11	106.97	118.30
2	H	229	H2U	P-O5'-C5'	-4.10	106.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	229	H2U	P-O5'-C5'	-4.10	107.00	118.30
2	L	229	H2U	P-O5'-C5'	-4.10	107.00	118.30
2	I	229	H2U	P-O5'-C5'	-4.09	107.04	118.30
2	E	229	H2U	P-O5'-C5'	-4.08	107.04	118.30
2	D	229	H2U	P-O5'-C5'	-4.05	107.14	118.30
2	J	229	H2U	P-O5'-C5'	-4.04	107.17	118.30
2	F	229	H2U	P-O5'-C5'	-4.04	107.18	118.30
2	M	229	H2U	P-O5'-C5'	-4.02	107.22	118.30
2	B	229	H2U	P-O5'-C5'	-4.01	107.24	118.30
2	C	229	H2U	P-O5'-C5'	-3.97	107.35	118.30
2	A	229	H2U	P-O5'-C5'	-3.88	107.61	118.30
2	C	229	H2U	O2-C2-N1	-3.01	119.35	123.12
2	A	229	H2U	O2-C2-N1	-2.99	119.37	123.12
2	M	229	H2U	O2-C2-N1	-2.99	119.37	123.12
2	K	229	H2U	O2-C2-N1	-2.99	119.37	123.12
2	F	229	H2U	O2-C2-N1	-2.98	119.38	123.12
2	J	229	H2U	O2-C2-N1	-2.98	119.38	123.12
2	I	229	H2U	O2-C2-N1	-2.97	119.39	123.12
2	L	229	H2U	O2-C2-N1	-2.97	119.39	123.12
2	D	229	H2U	O2-C2-N1	-2.97	119.40	123.12
2	B	229	H2U	O2-C2-N1	-2.95	119.42	123.12
2	G	229	H2U	O2-C2-N1	-2.94	119.44	123.12
2	E	229	H2U	O2-C2-N1	-2.94	119.44	123.12
2	H	229	H2U	O2-C2-N1	-2.93	119.44	123.12
2	C	229	H2U	C5-C4-N3	3.12	119.82	116.72
2	G	229	H2U	C5-C4-N3	3.15	119.86	116.72
2	K	229	H2U	C5-C4-N3	3.17	119.87	116.72
2	E	229	H2U	C5-C4-N3	3.21	119.91	116.72
2	B	229	H2U	C5-C4-N3	3.22	119.92	116.72
2	A	229	H2U	C5-C4-N3	3.22	119.93	116.72
2	H	229	H2U	C5-C4-N3	3.23	119.93	116.72
2	J	229	H2U	C5-C4-N3	3.25	119.95	116.72
2	F	229	H2U	C5-C4-N3	3.26	119.96	116.72
2	L	229	H2U	C5-C4-N3	3.26	119.97	116.72
2	D	229	H2U	C5-C4-N3	3.27	119.97	116.72
2	M	229	H2U	C5-C4-N3	3.29	119.99	116.72
2	I	229	H2U	C5-C4-N3	3.30	120.00	116.72
2	B	229	H2U	N3-C2-N1	4.76	121.47	116.73
2	E	229	H2U	N3-C2-N1	4.76	121.47	116.73
2	A	229	H2U	N3-C2-N1	4.77	121.48	116.73
2	G	229	H2U	N3-C2-N1	4.78	121.49	116.73
2	C	229	H2U	N3-C2-N1	4.84	121.55	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	229	H2U	N3-C2-N1	4.85	121.56	116.73
2	L	229	H2U	N3-C2-N1	4.86	121.57	116.73
2	F	229	H2U	N3-C2-N1	4.86	121.57	116.73
2	K	229	H2U	N3-C2-N1	4.88	121.59	116.73
2	I	229	H2U	N3-C2-N1	4.89	121.60	116.73
2	J	229	H2U	N3-C2-N1	4.90	121.61	116.73
2	H	229	H2U	N3-C2-N1	4.90	121.61	116.73
2	M	229	H2U	N3-C2-N1	4.91	121.61	116.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	229	H2U	1	0
2	D	229	H2U	2	0
2	F	229	H2U	1	0
2	G	229	H2U	1	0
2	I	229	H2U	2	0
2	M	229	H2U	2	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	221/228 (96%)	0.15	14 (6%) 21 27	26, 39, 59, 91	0
1	B	216/228 (94%)	0.33	19 (8%) 11 15	28, 47, 71, 102	0
1	C	218/228 (95%)	0.22	14 (6%) 20 26	29, 42, 71, 90	0
1	D	215/228 (94%)	0.62	21 (9%) 8 11	31, 52, 95, 124	0
1	E	217/228 (95%)	0.67	29 (13%) 4 5	46, 66, 85, 107	0
1	F	217/228 (95%)	0.58	28 (12%) 4 6	37, 62, 95, 114	0
1	G	217/228 (95%)	0.82	29 (13%) 4 5	50, 66, 105, 134	0
1	H	216/228 (94%)	0.73	26 (12%) 5 7	46, 67, 99, 124	0
1	I	212/228 (92%)	1.17	45 (21%) 1 1	36, 66, 139, 152	0
1	J	218/228 (95%)	0.45	17 (7%) 14 19	32, 58, 89, 112	0
1	K	216/228 (94%)	1.19	54 (25%) 1 1	62, 83, 103, 114	0
1	L	216/228 (94%)	1.17	46 (21%) 1 1	56, 90, 113, 130	0
1	M	217/228 (95%)	1.04	40 (18%) 1 2	33, 56, 86, 117	0
All	All	2816/2964 (95%)	0.70	382 (13%) 3 5	26, 61, 103, 152	0

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	225	LEU	9.6
1	I	159	THR	9.5
1	D	225	LEU	9.1
1	A	225	LEU	8.6
1	M	224	ASP	7.5
1	H	224	ASP	7.3
1	I	185	GLN	6.9
1	H	225	LEU	6.9
1	I	183	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
1	G	222	ILE	6.6
1	I	225	LEU	6.3
1	I	186	GLY	6.2
1	L	21	LEU	6.2
1	L	208	ALA	6.1
1	I	37	TYR	6.0
1	L	142	ILE	5.8
1	F	220	GLU	5.8
1	L	159	THR	5.8
1	I	181	GLY	5.7
1	L	161	PRO	5.7
1	G	208	ALA	5.7
1	K	74	ALA	5.5
1	A	5	ARG	5.4
1	I	223	LYS	5.4
1	F	218	ILE	5.2
1	I	164	LEU	5.2
1	G	209	ASP	5.2
1	L	193	LEU	5.1
1	L	207	LEU	5.1
1	H	223	LYS	5.1
1	I	189	PRO	5.1
1	I	217	GLY	5.1
1	D	222	ILE	5.1
1	M	195	PHE	5.0
1	K	224	ASP	5.0
1	G	207	LEU	4.9
1	I	207	LEU	4.9
1	B	222	ILE	4.9
1	L	222	ILE	4.9
1	I	209	ASP	4.9
1	A	7	ASP	4.9
1	I	184	ALA	4.8
1	M	9	MET	4.8
1	K	73	VAL	4.8
1	L	167	LEU	4.8
1	B	224	ASP	4.7
1	E	167	LEU	4.6
1	I	188	ASP	4.6
1	I	180	PRO	4.6
1	I	221	SER	4.6
1	L	211	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	209	ASP	4.5
1	D	208	ALA	4.5
1	J	225	LEU	4.5
1	G	218	ILE	4.5
1	K	147	VAL	4.5
1	E	96	ILE	4.4
1	M	14	ARG	4.4
1	I	222	ILE	4.4
1	G	225	LEU	4.4
1	M	223	LYS	4.4
1	L	224	ASP	4.4
1	I	182	VAL	4.3
1	H	181	GLY	4.3
1	K	206	TYR	4.3
1	I	194	ARG	4.2
1	K	195	PHE	4.2
1	D	224	ASP	4.2
1	K	216	ALA	4.2
1	H	37	TYR	4.2
1	F	207	LEU	4.1
1	E	97	VAL	4.1
1	K	220	GLU	4.1
1	H	187	GLY	4.1
1	K	207	LEU	4.1
1	L	164	LEU	4.0
1	E	224	ASP	4.0
1	J	224	ASP	4.0
1	L	221	SER	4.0
1	F	224	ASP	4.0
1	F	225	LEU	4.0
1	L	71	PHE	4.0
1	I	163	ARG	3.9
1	F	208	ALA	3.9
1	F	9	MET	3.9
1	I	162	GLU	3.9
1	L	195	PHE	3.9
1	D	11	VAL	3.9
1	G	206	TYR	3.8
1	K	15	LEU	3.8
1	F	217	GLY	3.8
1	B	109	CYS	3.8
1	K	120	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	223	LYS	3.8
1	M	100	PHE	3.8
1	H	222	ILE	3.8
1	K	97	VAL	3.8
1	K	189	PRO	3.8
1	K	208	ALA	3.7
1	K	96	ILE	3.7
1	I	220	GLU	3.7
1	K	222	ILE	3.7
1	G	224	ASP	3.7
1	G	23	ASN	3.7
1	H	219	ILE	3.7
1	K	152	LYS	3.7
1	J	159	THR	3.7
1	L	209	ASP	3.6
1	D	207	LEU	3.6
1	L	174	ASP	3.6
1	L	184	ALA	3.6
1	C	96	ILE	3.6
1	H	100	PHE	3.5
1	D	215	ALA	3.5
1	K	174	ASP	3.5
1	B	96	ILE	3.5
1	J	218	ILE	3.4
1	H	30	VAL	3.4
1	K	213	ALA	3.4
1	E	66	ARG	3.4
1	G	221	SER	3.4
1	G	41	VAL	3.4
1	I	166	ARG	3.4
1	K	167	LEU	3.4
1	H	74	ALA	3.3
1	B	37	TYR	3.3
1	M	222	ILE	3.3
1	D	211	PRO	3.3
1	A	6	VAL	3.3
1	M	96	ILE	3.3
1	A	224	ASP	3.3
1	K	182	VAL	3.3
1	D	220	GLU	3.3
1	H	123	LEU	3.2
1	K	183	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	71	PHE	3.2
1	K	193	LEU	3.2
1	H	186	GLY	3.2
1	G	188	ASP	3.2
1	M	97	VAL	3.2
1	L	194	ARG	3.2
1	M	43	ILE	3.1
1	E	100	PHE	3.1
1	K	225	LEU	3.1
1	A	96	ILE	3.1
1	I	22	MET	3.1
1	L	206	TYR	3.1
1	I	36	GLU	3.1
1	F	222	ILE	3.1
1	I	187	GLY	3.1
1	C	66	ARG	3.1
1	C	69	ALA	3.1
1	L	196	ALA	3.1
1	B	220	GLU	3.1
1	H	73	VAL	3.0
1	G	38	ILE	3.0
1	L	214	ALA	3.0
1	C	73	VAL	3.0
1	I	160	ARG	3.0
1	J	191	GLU	3.0
1	E	216	ALA	3.0
1	L	205	ILE	3.0
1	J	97	VAL	3.0
1	G	74	ALA	2.9
1	I	218	ILE	2.9
1	C	74	ALA	2.9
1	C	68	ILE	2.9
1	D	96	ILE	2.9
1	C	37	TYR	2.9
1	H	208	ALA	2.9
1	K	21	LEU	2.9
1	F	74	ALA	2.9
1	I	208	ALA	2.9
1	K	95	ILE	2.9
1	F	23	ASN	2.9
1	G	160	ARG	2.9
1	L	25	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	192	THR	2.8
1	L	152	LYS	2.8
1	M	189	PRO	2.8
1	C	70	ASP	2.8
1	M	66	ARG	2.8
1	M	166	ARG	2.8
1	M	194	ARG	2.8
1	B	225	LEU	2.8
1	H	97	VAL	2.8
1	I	191	GLU	2.8
1	C	155	VAL	2.8
1	M	72	LYS	2.8
1	H	69	ALA	2.8
1	L	15	LEU	2.8
1	L	223	LYS	2.8
1	J	96	ILE	2.8
1	K	214	ALA	2.7
1	I	96	ILE	2.7
1	K	72	LYS	2.7
1	E	69	ALA	2.7
1	C	72	LYS	2.7
1	J	166	ARG	2.7
1	K	166	ARG	2.7
1	I	199	ILE	2.7
1	E	173	GLN	2.7
1	F	22	MET	2.7
1	M	209	ASP	2.7
1	K	107	ARG	2.7
1	E	74	ALA	2.7
1	L	107	ARG	2.7
1	C	97	VAL	2.7
1	G	211	PRO	2.7
1	F	209	ASP	2.7
1	K	162	GLU	2.7
1	K	149	LEU	2.7
1	F	211	PRO	2.6
1	E	25	ASP	2.6
1	E	210	ASN	2.6
1	G	96	ILE	2.6
1	K	169	GLU	2.6
1	H	27	ALA	2.6
1	E	225	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	71	PHE	2.6
1	K	103	ALA	2.6
1	K	14	ARG	2.6
1	J	223	LYS	2.6
1	K	223	LYS	2.6
1	M	73	VAL	2.6
1	G	166	ARG	2.6
1	E	68	ILE	2.6
1	H	96	ILE	2.6
1	M	10	ASP	2.6
1	K	173	GLN	2.6
1	E	73	VAL	2.6
1	E	191	GLU	2.6
1	B	191	GLU	2.6
1	B	72	LYS	2.6
1	G	223	LYS	2.6
1	K	124	THR	2.5
1	G	187	GLY	2.5
1	B	74	ALA	2.5
1	L	23	ASN	2.5
1	M	214	ALA	2.5
1	E	217	GLY	2.5
1	M	174	ASP	2.5
1	B	71	PHE	2.5
1	A	69	ALA	2.5
1	M	45	TYR	2.5
1	F	72	LYS	2.5
1	M	207	LEU	2.5
1	E	195	PHE	2.5
1	L	100	PHE	2.5
1	I	169	GLU	2.5
1	H	72	LYS	2.5
1	L	43	ILE	2.5
1	C	123	LEU	2.5
1	L	28	LEU	2.5
1	M	167	LEU	2.5
1	I	34	VAL	2.4
1	M	217	GLY	2.4
1	K	85	ARG	2.4
1	H	36	GLU	2.4
1	M	36	GLU	2.4
1	D	223	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	74	ALA	2.4
1	G	219	ILE	2.4
1	H	162	GLU	2.4
1	D	214	ALA	2.4
1	G	73	VAL	2.4
1	M	37	TYR	2.4
1	E	26	ASP	2.4
1	I	224	ASP	2.4
1	K	61	LYS	2.4
1	L	37	TYR	2.4
1	M	68	ILE	2.4
1	B	162	GLU	2.4
1	M	122	LEU	2.4
1	L	74	ALA	2.4
1	L	202	GLY	2.4
1	F	73	VAL	2.4
1	K	65	CYS	2.4
1	L	220	GLU	2.4
1	L	29	ARG	2.4
1	L	160	ARG	2.4
1	I	210	ASN	2.4
1	H	214	ALA	2.3
1	J	194	ARG	2.3
1	D	38	ILE	2.3
1	L	169	GLU	2.3
1	F	223	LYS	2.3
1	A	71	PHE	2.3
1	L	183	GLY	2.3
1	I	157	PRO	2.3
1	K	171	ILE	2.3
1	D	37	TYR	2.3
1	G	22	MET	2.3
1	F	34	VAL	2.3
1	B	36	GLU	2.3
1	H	67	ILE	2.3
1	I	213	ALA	2.3
1	K	164	LEU	2.3
1	B	73	VAL	2.3
1	L	171	ILE	2.3
1	E	98	HIS	2.2
1	E	218	ILE	2.2
1	G	67	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	28	LEU	2.2
1	I	152	LYS	2.2
1	E	209	ASP	2.2
1	K	212	ALA	2.2
1	K	191	GLU	2.2
1	M	132	GLU	2.2
1	M	61	LYS	2.2
1	C	71	PHE	2.2
1	A	74	ALA	2.2
1	I	69	ALA	2.2
1	J	69	ALA	2.2
1	F	96	ILE	2.2
1	J	95	ILE	2.2
1	K	67	ILE	2.2
1	F	191	GLU	2.2
1	L	58	GLU	2.2
1	D	162	GLU	2.2
1	K	161	PRO	2.2
1	F	63	PHE	2.2
1	J	173	GLN	2.2
1	M	98	HIS	2.2
1	E	95	ILE	2.2
1	A	123	LEU	2.2
1	D	123	LEU	2.2
1	F	15	LEU	2.2
1	L	189	PRO	2.2
1	B	223	LYS	2.1
1	D	183	GLY	2.2
1	E	34	VAL	2.1
1	M	62	ARG	2.1
1	G	191	GLU	2.1
1	A	73	VAL	2.1
1	I	23	ASN	2.1
1	K	105	SER	2.1
1	F	213	ALA	2.1
1	K	69	ALA	2.1
1	M	206	TYR	2.1
1	A	68	ILE	2.1
1	G	200	ILE	2.1
1	H	13	ASN	2.1
1	H	221	SER	2.1
1	L	62	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	123	LEU	2.1
1	E	43	ILE	2.1
1	B	69	ALA	2.1
1	C	213	ALA	2.1
1	M	94	ALA	2.1
1	M	120	VAL	2.1
1	K	100	PHE	2.1
1	G	189	PRO	2.1
1	B	95	ILE	2.1
1	B	218	ILE	2.1
1	M	67	ILE	2.1
1	B	98	HIS	2.1
1	E	70	ASP	2.1
1	J	220	GLU	2.1
1	A	97	VAL	2.1
1	L	155	VAL	2.1
1	D	16	ILE	2.0
1	G	194	ARG	2.0
1	J	207	LEU	2.0
1	D	97	VAL	2.0
1	F	30	VAL	2.0
1	F	206	TYR	2.0
1	E	72	LYS	2.0
1	D	40	THR	2.0
1	J	217	GLY	2.0
1	M	44	GLY	2.0
1	E	212	ALA	2.0
1	A	174	ASP	2.0
1	G	39	ASP	2.0
1	K	194	ARG	2.0
1	K	203	ARG	2.0
1	F	97	VAL	2.0
1	K	176	PHE	2.0
1	F	123	LEU	2.0
1	F	193	LEU	2.0
1	I	200	ILE	2.0
1	J	183	GLY	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 [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	H2U	L	229	21/21	0.73	0.25	0.63	118,119,123,124	0
2	H2U	C	229	21/21	0.94	0.21	0.48	37,39,48,51	0
2	H2U	J	229	21/21	0.89	0.20	0.47	64,67,69,70	0
2	H2U	A	229	21/21	0.96	0.18	0.42	31,37,40,43	0
2	H2U	I	229	21/21	0.63	0.33	0.39	137,138,138,139	0
2	H2U	F	229	21/21	0.80	0.17	-0.01	57,64,69,70	0
2	H2U	B	229	21/21	0.94	0.15	-0.05	42,45,52,54	0
2	H2U	G	229	21/21	0.91	0.17	-0.15	64,66,75,76	0
2	H2U	E	229	21/21	0.94	0.16	-0.23	57,59,64,64	0
2	H2U	M	229	21/21	0.89	0.18	-0.37	59,66,68,70	0
2	H2U	K	229	21/21	0.89	0.16	-0.41	72,75,77,78	0
2	H2U	H	229	21/21	0.93	0.13	-0.89	64,68,78,79	0
2	H2U	D	229	21/21	0.92	0.14	-0.90	54,58,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.