



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:29 am GMT

PDB ID : 4E1V
Title : X-RAY Structure of the Uridine Phosphorylase from Salmonella Typhimurium
in Complex with 5-Fluorouracil at 2.15 Å Resolution
Authors : Lashkov, A.A.; Sotnichenko, S.E.; Prokofev, I.I.; Gabdoulkhakov, A.G.;
Mikhailov, A.M.
Deposited on : 2012-03-07
Resolution : 2.15 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:

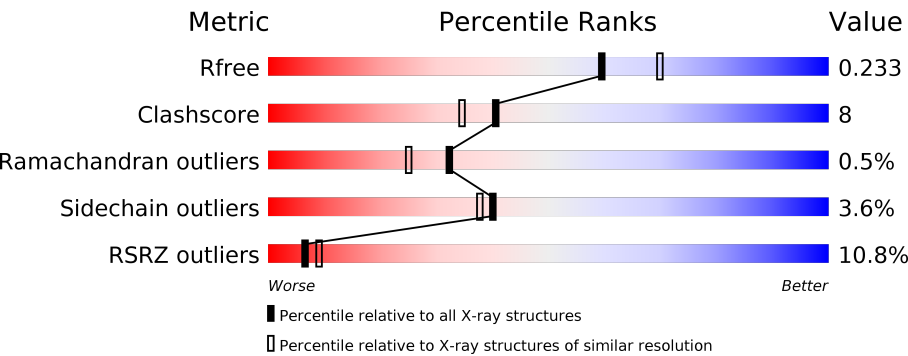
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	253	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>76%20% . .</div></div>
1	B	253	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>85%10% . .</div></div>
1	C	253	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>84%12% . .</div></div>
1	D	253	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>84%13% .</div></div>
1	E	253	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>87%8% . .</div></div>
1	F	253	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>86%9% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	253	
1	H	253	
1	I	253	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URF	G	1301	-	X	-	-
2	URF	H	1301	-	X	-	-
3	GOL	A	1302	-	-	-	X
3	GOL	B	1302	-	-	-	X
3	GOL	C	1303	-	-	-	X
3	GOL	E	1302	-	-	-	X
3	GOL	F	1302	-	-	-	X
4	K	D	1302	-	-	-	X
5	EDO	C	1302	-	-	X	-

2 Entry composition

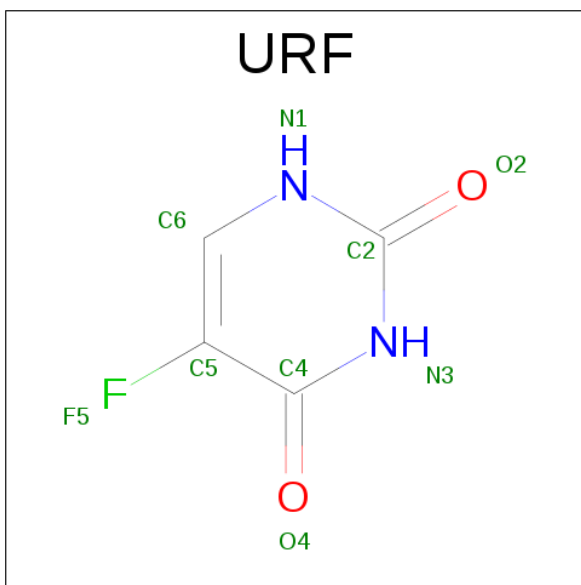
There are 6 unique types of molecules in this entry. The entry contains 17042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	1	0
			1868	1171	330	356	11			
1	E	245	Total	C	N	O	S	0	0	0
			1835	1149	323	352	11			
1	F	242	Total	C	N	O	S	0	0	0
			1814	1137	320	346	11			
1	D	245	Total	C	N	O	S	0	1	0
			1843	1156	325	351	11			
1	C	246	Total	C	N	O	S	0	0	0
			1846	1156	325	354	11			
1	B	244	Total	C	N	O	S	0	1	0
			1838	1153	324	350	11			
1	H	243	Total	C	N	O	S	0	0	0
			1824	1143	321	349	11			
1	I	243	Total	C	N	O	S	0	0	0
			1823	1143	322	347	11			
1	G	242	Total	C	N	O	S	0	0	0
			1814	1137	320	346	11			

- Molecule 2 is 5-FLUOROURACIL (three-letter code: URF) (formula: C₄H₃FN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	E	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	F	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	D	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	C	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	B	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	H	1	Total	C	F	N	O	0	0
			9	4	1	2	2		
2	G	1	Total	C	F	N	O	0	0
			9	4	1	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

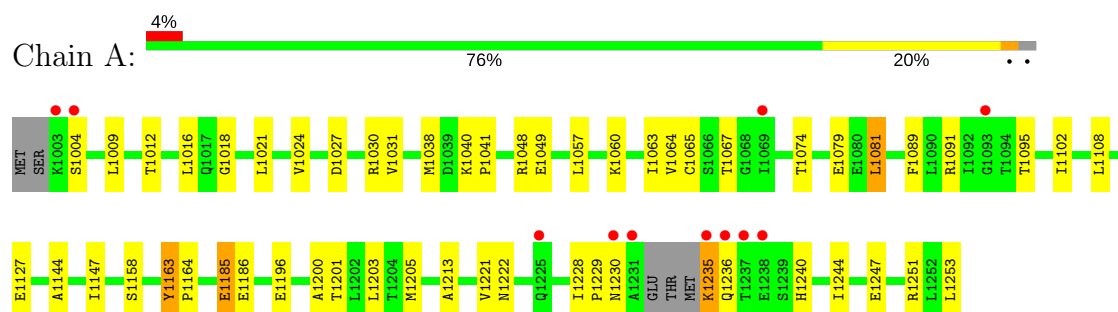
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total	O	0	1
			62	62		
6	E	62	Total	O	0	0
			62	62		
6	F	67	Total	O	0	0
			67	67		
6	D	69	Total	O	0	1
			70	70		
6	C	58	Total	O	0	0
			58	58		
6	B	66	Total	O	0	0
			66	66		
6	H	16	Total	O	0	0
			16	16		
6	I	12	Total	O	0	0
			12	12		
6	G	15	Total	O	0	0
			15	15		

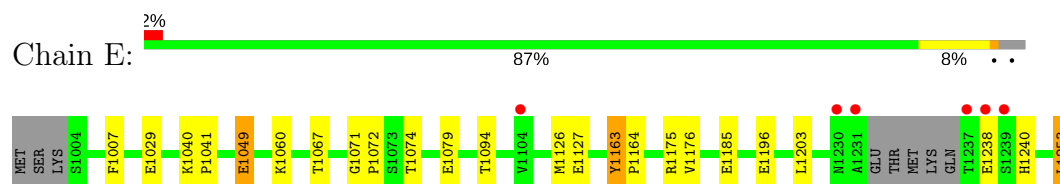
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

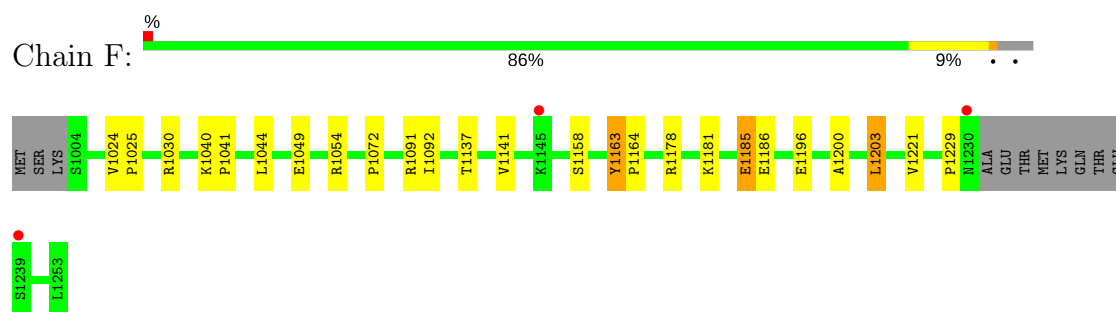
- Molecule 1: Uridine phosphorylase



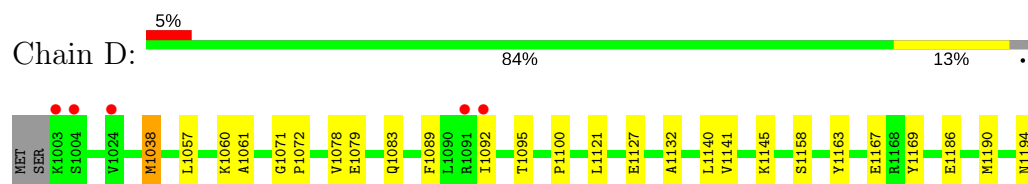
- Molecule 1: Uridine phosphorylase

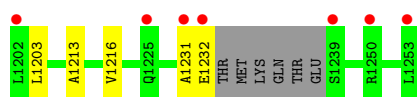


- Molecule 1: Uridine phosphorylase

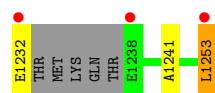
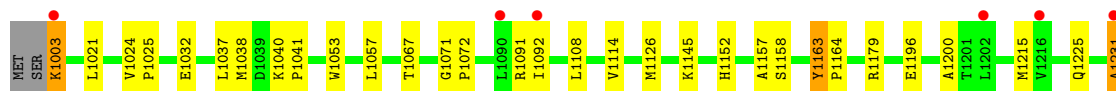
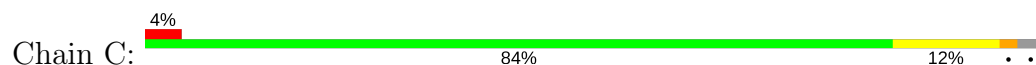


- Molecule 1: Uridine phosphorylase

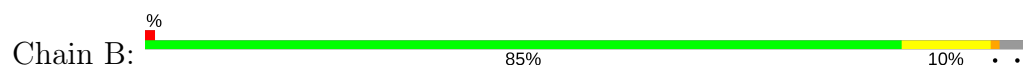




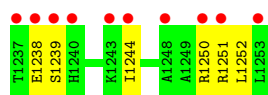
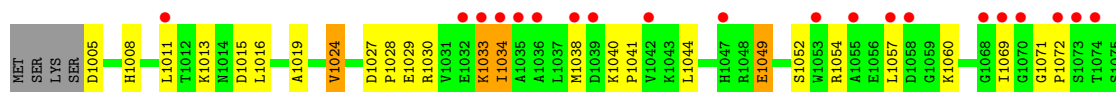
- Molecule 1: Uridine phosphorylase



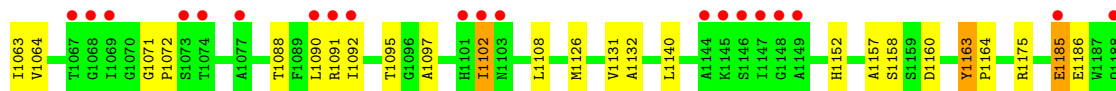
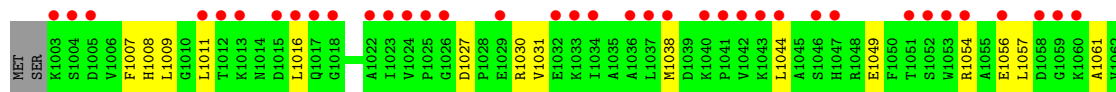
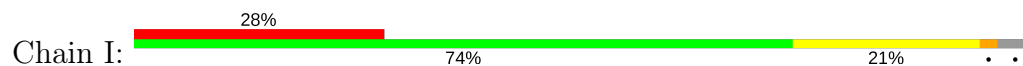
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase

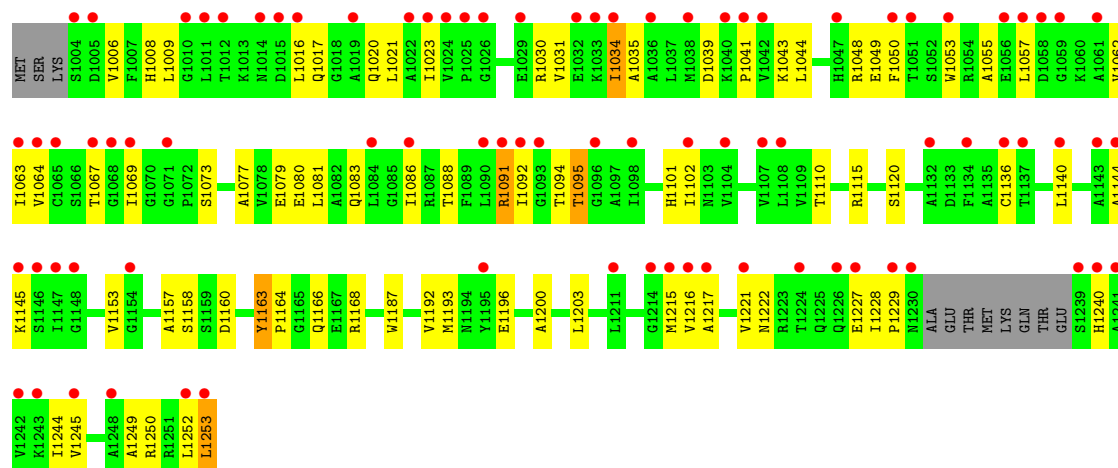


- Molecule 1: Uridine phosphorylase





• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.49Å 93.21Å 149.97Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	28.88 – 2.15 29.53 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.9 (28.88-2.15) 96.9 (29.53-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.194 , 0.238 0.189 , 0.233	Depositor DCC
R_{free} test set	5748 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.026 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.077 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.057 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: GOL, URF, K, EDO

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	0.37	0/1900	0.52	0/2571
1	B	0.38	0/1870	0.53	0/2531
1	C	0.38	0/1875	0.53	0/2539
1	D	0.40	0/1875	0.54	0/2538
1	E	0.37	0/1864	0.53	0/2526
1	F	0.37	0/1843	0.53	0/2497
1	G	0.28	0/1843	0.48	0/2497
1	H	0.31	0/1853	0.48	0/2511
1	I	0.26	0/1852	0.45	0/2508
All	All	0.35	0/16775	0.51	0/22718

There are no bond length outliers.

There are no bond angle outliers.

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	1868	0	1890	38	0
1	B	1838	0	1857	18	0
1	C	1846	0	1855	23	0
1	D	1843	0	1862	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1835	0	1843	20	0
1	F	1814	0	1825	25	0
1	G	1814	0	1825	69	0
1	H	1824	0	1833	39	0
1	I	1823	0	1838	34	0
2	A	9	0	3	1	0
2	B	9	0	3	2	0
2	C	9	0	3	2	0
2	D	9	0	3	0	0
2	E	9	0	3	1	0
2	F	9	0	3	1	0
2	G	9	0	3	0	0
2	H	9	0	3	0	0
3	A	6	0	8	1	0
3	B	6	0	8	3	0
3	C	6	0	8	2	0
3	E	6	0	8	2	0
3	F	6	0	8	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	C	4	0	6	4	0
6	A	62	0	0	0	0
6	B	66	0	0	1	0
6	C	58	0	0	0	0
6	D	70	0	0	1	0
6	E	62	0	0	0	0
6	F	67	0	0	1	0
6	G	15	0	0	0	0
6	H	16	0	0	0	0
6	I	12	0	0	1	0
All	All	17042	0	16698	274	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 8.

All (274) 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:G:1095:THR:CG2	1:G:1217:ALA:HB1	1.97	0.94
2:E:1301:URF:HN1	3:E:1302:GOL:H2	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1069:ILE:HD11	1:G:1048:ARG:HD3	1.55	0.88
1:G:1021:LEU:HD21	1:G:1088:THR:HB	1.59	0.84
1:I:1163:TYR:HB2	1:I:1164:PRO:HD3	1.61	0.83
1:G:1095:THR:HG22	1:G:1217:ALA:HB1	1.60	0.82
1:G:1095:THR:HG21	1:G:1217:ALA:CB	2.10	0.82
2:A:1301:URF:HN1	3:A:1302:GOL:H2	1.51	0.75
1:G:1055:ALA:O	1:G:1062:VAL:N	2.20	0.75
1:C:1179:ARG:HD2	5:C:1302:EDO:H21	1.68	0.74
1:H:1016:LEU:HG	1:H:1019:ALA:HB3	1.70	0.74
1:G:1166:GLN:OE1	1:G:1168:ARG:NH1	2.22	0.72
1:G:1020:GLN:C	1:G:1021:LEU:HD12	2.09	0.72
1:G:1020:GLN:O	1:G:1021:LEU:HD12	1.88	0.71
1:F:1158:SER:HB3	1:F:1200:ALA:HB2	1.71	0.71
1:H:1144:ALA:HA	1:H:1244:ILE:HD12	1.72	0.71
1:C:1067:THR:OG1	1:C:1091:ARG:NH1	2.24	0.70
1:I:1228:ILE:HB	1:I:1229:PRO:HD2	1.73	0.69
1:G:1006:VAL:HG11	1:G:1080:GLU:O	1.94	0.68
1:A:1144:ALA:HA	1:A:1244:ILE:HD12	1.76	0.68
1:G:1021:LEU:HD21	1:G:1088:THR:CB	2.25	0.67
1:G:1081:LEU:HB3	1:G:1086:ILE:HD12	1.75	0.67
1:G:1031:VAL:HG13	1:G:1064:VAL:HG12	1.75	0.67
1:E:1049:GLU:HB3	1:F:1049:GLU:HG2	1.78	0.66
1:D:1167:GLU:HG2	1:D:1169:TYR:CE1	2.32	0.65
1:A:1024:VAL:O	1:A:1091:ARG:HD2	1.96	0.65
1:F:1221:VAL:HB	1:F:1229:PRO:HB3	1.78	0.65
1:I:1044:LEU:HD11	1:I:1054:ARG:HB2	1.79	0.65
1:G:1021:LEU:CD2	1:G:1088:THR:HB	2.26	0.65
1:G:1095:THR:HG21	1:G:1217:ALA:HB1	1.67	0.65
1:H:1033:LYS:HA	1:H:1033:LYS:HE3	1.78	0.65
1:I:1228:ILE:HB	1:I:1229:PRO:CD	2.28	0.64
1:G:1101:HIS:O	1:G:1102:ILE:HD12	1.98	0.64
1:D:1231:ALA:O	1:D:1232:GLU:HB3	1.97	0.64
1:G:1095:THR:HG21	1:G:1217:ALA:HB3	1.79	0.63
1:G:1034:ILE:HG22	1:G:1064:VAL:HG21	1.80	0.63
1:A:1018:GLY:O	1:A:1060[A]:LYS:NZ	2.33	0.62
1:G:1102:ILE:O	1:G:1222:ASN:ND2	2.33	0.62
1:C:1092:ILE:HD11	1:C:1241:ALA:HB1	1.81	0.61
1:G:1101:HIS:ND1	1:G:1102:ILE:HD12	2.14	0.61
2:C:1301:URF:HN1	3:C:1303:GOL:H2	1.65	0.61
1:G:1158:SER:HB3	1:G:1200:ALA:HB2	1.83	0.61
1:G:1031:VAL:HG13	1:G:1064:VAL:CG1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:HIS:O	1:A:1244:ILE:HG12	2.00	0.60
1:C:1179:ARG:NH1	5:C:1302:EDO:O1	2.34	0.60
1:D:1121:LEU:HD22	5:C:1302:EDO:H12	1.82	0.60
1:A:1144:ALA:HA	1:A:1244:ILE:CD1	2.31	0.60
1:G:1034:ILE:HG22	1:G:1035:ALA:N	2.17	0.59
1:G:1020:GLN:O	1:G:1086:ILE:HG23	2.03	0.59
1:G:1021:LEU:HD21	1:G:1088:THR:CG2	2.32	0.59
1:I:1158:SER:HB3	1:I:1200:ALA:HB2	1.84	0.59
2:F:1301:URF:HN1	3:F:1302:GOL:H11	1.67	0.57
1:I:1090:LEU:HD11	1:I:1252:LEU:HD12	1.86	0.57
1:E:1094:THR:HG1	3:E:1302:GOL:HO2	1.49	0.57
1:F:1044:LEU:HD11	1:F:1054:ARG:HB2	1.86	0.57
1:D:1100:PRO:HG2	6:D:1465:HOH:O	2.05	0.57
1:G:1101:HIS:ND1	1:G:1102:ILE:CD1	2.67	0.57
1:D:1038:MET:HB3	1:D:1057:LEU:HD13	1.87	0.56
1:H:1028:PRO:HD2	1:G:1048:ARG:HA	1.87	0.56
1:G:1101:HIS:C	1:G:1102:ILE:HD12	2.27	0.56
1:A:1004:SER:HA	1:A:1012:THR:HG22	1.87	0.55
1:D:1140:LEU:HD22	1:D:1216:VAL:HB	1.88	0.55
1:F:1054:ARG:NH2	6:F:1434:HOH:O	2.38	0.55
1:H:1109:VAL:HB	1:H:1153:VAL:HG22	1.88	0.55
1:C:1158:SER:HB3	1:C:1200:ALA:HB2	1.89	0.55
1:E:1049:GLU:HG2	1:F:1049:GLU:HG2	1.88	0.55
1:G:1016:LEU:O	1:G:1017:GLN:HB2	2.06	0.55
1:C:1179:ARG:CD	5:C:1302:EDO:H21	2.34	0.55
1:G:1044:LEU:HD11	1:G:1063:ILE:CD1	2.37	0.55
1:E:1060:LYS:HD2	1:E:1253:LEU:HB3	1.87	0.55
1:G:1163:TYR:HB2	1:G:1164:PRO:HD3	1.88	0.55
1:D:1167:GLU:HG2	1:D:1169:TYR:HE1	1.70	0.55
1:F:1163:TYR:HB2	1:F:1164:PRO:CD	2.36	0.55
1:G:1021:LEU:HG	1:G:1088:THR:O	2.07	0.55
1:E:1040:LYS:N	1:E:1041:PRO:HD3	2.22	0.54
1:H:1005:ASP:OD2	1:H:1005:ASP:N	2.40	0.54
1:C:1108:LEU:HD22	1:C:1152:HIS:HB2	1.89	0.54
1:H:1005:ASP:N	1:H:1011:LEU:O	2.41	0.54
1:H:1163:TYR:HB2	1:H:1164:PRO:CD	2.38	0.54
1:G:1021:LEU:CG	1:G:1088:THR:HB	2.38	0.54
1:H:1076:ILE:HD12	1:G:1069:ILE:HD13	1.89	0.53
1:H:1168:ARG:HG2	1:H:1227:GLU:HG3	1.91	0.53
1:E:1163:TYR:HB2	1:E:1164:PRO:CD	2.37	0.53
1:A:1040:LYS:N	1:A:1041:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1040:LYS:N	1:F:1041:PRO:HD3	2.24	0.53
1:E:1175:ARG:HG2	1:E:1176:VAL:N	2.24	0.53
1:G:1094:THR:C	1:G:1095:THR:HG22	2.29	0.53
1:H:1040:LYS:N	1:H:1041:PRO:HD3	2.23	0.53
1:H:1252:LEU:O	1:H:1252:LEU:HD12	2.09	0.53
1:C:1071:GLY:N	1:C:1072:PRO:CD	2.72	0.52
1:G:1030:ARG:O	1:G:1034:ILE:HD12	2.09	0.52
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.91	0.52
1:D:1060[B]:LYS:HD2	1:D:1061:ALA:N	2.25	0.52
1:I:1102:ILE:HD12	1:I:1108:LEU:HD21	1.91	0.52
1:C:1091:ARG:HG2	1:C:1215:MET:SD	2.50	0.52
1:H:1163:TYR:CB	1:H:1164:PRO:CD	2.88	0.52
1:B:1116:LEU:HB2	1:B:1158:SER:O	2.10	0.52
1:D:1060[A]:LYS:HD3	1:D:1061:ALA:N	2.24	0.52
1:A:1027:ASP:HB3	1:A:1030:ARG:HG3	1.91	0.51
1:B:1163:TYR:HB2	1:B:1164:PRO:CD	2.40	0.51
1:B:1163:TYR:CB	1:B:1164:PRO:CD	2.88	0.51
1:I:1071:GLY:N	1:I:1072:PRO:CD	2.74	0.51
1:F:1137:THR:O	1:F:1141:VAL:HG23	2.10	0.51
1:G:1110:THR:HB	1:G:1215:MET:HB3	1.92	0.51
1:A:1038:MET:HG2	1:A:1057:LEU:HD13	1.93	0.51
1:E:1007:PHE:CE1	1:F:1229:PRO:HG2	2.46	0.51
1:H:1049:GLU:CD	1:G:1069:ILE:H	2.15	0.51
1:I:1016:LEU:HG	1:I:1063:ILE:HD12	1.93	0.50
1:B:1054:ARG:HG2	6:B:1406:HOH:O	2.11	0.50
1:I:1229:PRO:O	1:I:1230:ASN:CB	2.59	0.50
1:I:1088:THR:HA	1:I:1212:ARG:HB2	1.94	0.50
1:G:1250:ARG:HA	1:G:1253:LEU:HD22	1.92	0.50
1:H:1125:PRO:HB2	1:H:1127:GLU:OE2	2.12	0.50
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.42	0.49
1:I:1038:MET:HG2	1:I:1057:LEU:HD12	1.94	0.49
1:D:1079:GLU:O	1:D:1083:GLN:HG3	2.13	0.49
1:A:1095:THR:HG21	1:A:1108:LEU:HD12	1.94	0.49
1:B:1158:SER:HB3	1:B:1200:ALA:HB2	1.95	0.49
1:G:1163:TYR:HB2	1:G:1164:PRO:CD	2.43	0.48
1:H:1071:GLY:N	1:H:1072:PRO:CD	2.76	0.48
1:G:1067:THR:O	1:G:1073:SER:HB3	2.13	0.48
1:H:1091:ARG:HG3	1:H:1202:LEU:HD22	1.95	0.48
1:A:1009:LEU:CD1	1:A:1081:LEU:HD13	2.44	0.48
1:F:1163:TYR:CB	1:F:1164:PRO:CD	2.91	0.48
1:I:1071:GLY:N	1:I:1072:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:ASN:HB2	1:A:1235:LYS:CE	2.44	0.48
1:F:1092:ILE:O	1:F:1092:ILE:HG23	2.12	0.48
1:H:1027:ASP:OD2	1:H:1029:GLU:HB2	2.13	0.48
1:E:1127:GLU:CD	1:E:1127:GLU:H	2.17	0.48
1:B:1044:LEU:HD11	1:B:1054:ARG:HB2	1.96	0.48
1:F:1024:VAL:O	1:F:1091:ARG:HD2	2.13	0.48
1:G:1030:ARG:O	1:G:1034:ILE:CD1	2.62	0.48
1:G:1030:ARG:HB3	1:G:1034:ILE:CD1	2.44	0.48
1:A:1102:ILE:O	1:A:1222:ASN:ND2	2.47	0.47
1:G:1008:HIS:H	1:G:1080:GLU:CD	2.17	0.47
1:G:1240:HIS:O	1:G:1244:ILE:HG12	2.14	0.47
1:D:1089:PHE:O	1:D:1213:ALA:HA	2.12	0.47
1:B:1090:LEU:HD11	1:B:1252:LEU:HD12	1.95	0.47
1:G:1221:VAL:HB	1:G:1229:PRO:HB3	1.97	0.47
1:G:1168:ARG:HE	1:G:1227:GLU:HB2	1.80	0.47
1:I:1095:THR:OG1	1:I:1194:ASN:HB2	2.14	0.47
1:A:1016:LEU:HG	1:A:1063:ILE:HG13	1.96	0.47
1:I:1057:LEU:HD21	1:I:1250:ARG:HB3	1.96	0.47
1:A:1009:LEU:HD12	1:A:1081:LEU:HD13	1.97	0.47
1:D:1158:SER:HB3	1:D:1200:ALA:HB2	1.97	0.47
1:E:1071:GLY:N	1:E:1072:PRO:CD	2.78	0.47
1:E:1049:GLU:CB	1:F:1049:GLU:HG2	2.45	0.47
1:A:1163:TYR:HB2	1:A:1164:PRO:HD3	1.96	0.46
1:B:1247:GLU:HG3	1:B:1251:ARG:HH22	1.80	0.46
1:C:1038:MET:HE2	1:C:1057:LEU:HB2	1.97	0.46
1:H:1015:ASP:O	1:H:1054:ARG:NE	2.47	0.46
1:H:1147:ILE:HG13	1:H:1244:ILE:HD13	1.98	0.46
1:E:1067:THR:HB	1:E:1074:THR:HA	1.98	0.46
1:E:1238:GLU:O	1:E:1238:GLU:HG3	2.15	0.46
1:H:1008:HIS:CE1	1:H:1076:ILE:HD13	2.51	0.46
1:I:1027:ASP:HB3	1:I:1030:ARG:HB2	1.98	0.46
1:D:1132:ALA:HA	1:D:1203:LEU:HD22	1.97	0.46
1:C:1231:ALA:O	1:C:1232:GLU:HB3	2.15	0.46
1:F:1163:TYR:HB2	1:F:1164:PRO:HD3	1.98	0.46
1:H:1169:TYR:O	1:H:1171:THR:N	2.49	0.46
1:A:1163:TYR:CB	1:A:1164:PRO:CD	2.93	0.46
1:I:1221:VAL:HG22	1:I:1222:ASN:N	2.31	0.46
1:I:1031:VAL:HG13	1:I:1064:VAL:HG12	1.98	0.46
1:A:1067:THR:OG1	1:A:1091:ARG:NH1	2.46	0.45
1:I:1092:ILE:HA	1:I:1216:VAL:O	2.16	0.45
1:C:1057:LEU:HB3	1:C:1253:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1196:GLU:CD	1:I:1198:GLU:H	2.19	0.45
1:A:1147:ILE:O	1:A:1147:ILE:HG22	2.15	0.45
1:A:1185:GLU:HG3	1:A:1186:GLU:N	2.31	0.45
1:A:1247:GLU:HG3	1:A:1251:ARG:HH12	1.82	0.45
1:G:1023:ILE:HD12	1:G:1245:VAL:HG22	1.99	0.45
1:H:1024:VAL:HG23	1:H:1091:ARG:HA	1.99	0.45
1:D:1186:GLU:O	1:D:1190:MET:HG3	2.16	0.45
1:G:1041:PRO:HB2	1:G:1053:TRP:CZ3	2.52	0.45
1:I:1011:LEU:HD11	1:I:1044:LEU:HD13	1.98	0.45
1:C:1040:LYS:N	1:C:1041:PRO:CD	2.80	0.45
1:F:1181:LYS:O	1:B:1178:ARG:NH2	2.50	0.45
1:A:1127:GLU:CD	1:A:1127:GLU:H	2.21	0.45
1:G:1157:ALA:HB2	1:G:1192:VAL:HG11	1.99	0.45
1:H:1163:TYR:HB2	1:H:1164:PRO:HD3	1.98	0.45
1:I:1009:LEU:HB3	1:I:1011:LEU:HD23	1.99	0.44
1:C:1163:TYR:HB2	1:C:1164:PRO:CD	2.47	0.44
1:H:1108:LEU:HD22	1:H:1152:HIS:HB2	1.99	0.44
1:H:1049:GLU:HG2	1:G:1049:GLU:HB3	1.99	0.44
1:G:1095:THR:CG2	1:G:1217:ALA:CB	2.71	0.44
1:B:1108:LEU:HD22	1:B:1152:HIS:HB2	2.00	0.44
1:E:1163:TYR:CB	1:E:1164:PRO:CD	2.95	0.44
1:H:1251:ARG:HD3	1:H:1251:ARG:HA	1.76	0.44
1:B:1197:MET:HB2	3:B:1302:GOL:O3	2.18	0.44
1:B:1071:GLY:N	1:B:1072:PRO:CD	2.81	0.44
1:D:1141:VAL:O	1:D:1145:LYS:HG2	2.18	0.44
1:G:1023:ILE:HD11	1:G:1249:ALA:HB2	2.00	0.44
1:C:1024:VAL:HA	1:C:1025:PRO:HD2	1.91	0.44
1:I:1131:VAL:HG22	1:I:1132:ALA:O	2.18	0.44
1:D:1071:GLY:N	1:D:1072:PRO:CD	2.81	0.43
1:B:1170:ASP:HA	1:H:1013:LYS:HD3	1.99	0.43
1:A:1067:THR:HB	1:A:1074:THR:HA	2.00	0.43
1:A:1201:THR:O	1:A:1205:MET:HG2	2.19	0.43
1:D:1078:VAL:HG13	1:D:1089:PHE:CZ	2.54	0.43
1:G:1145:LYS:HB3	1:G:1145:LYS:HE3	1.87	0.43
1:I:1185:GLU:HG2	1:I:1186:GLU:N	2.32	0.43
1:A:1048:ARG:HB3	1:A:1049:GLU:OE1	2.18	0.43
1:E:1049:GLU:HB3	1:F:1049:GLU:CG	2.47	0.43
1:H:1126:MET:HG3	1:I:1126:MET:HG3	2.01	0.43
1:I:1097:ALA:HB2	1:I:1102:ILE:HD11	2.00	0.43
1:G:1091:ARG:HG2	1:G:1215:MET:SD	2.58	0.43
1:G:1136:CYS:HA	1:G:1252:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:GLU:OE2	1:B:1199:SER:OG	2.34	0.43
1:G:1044:LEU:CD1	1:G:1063:ILE:HD12	2.49	0.43
1:G:1057:LEU:HB3	1:G:1253:LEU:HD21	2.00	0.43
1:E:1079:GLU:HG2	1:F:1163:TYR:CD2	2.54	0.43
1:H:1038:MET:SD	1:H:1057:LEU:HD11	2.58	0.43
2:B:1301:URF:HN1	3:B:1302:GOL:H31	1.84	0.43
1:C:1021:LEU:HD13	1:C:1253:LEU:CD1	2.49	0.43
1:A:1221:VAL:HB	1:A:1229:PRO:HG3	2.01	0.43
2:B:1301:URF:HN1	3:B:1302:GOL:C3	2.32	0.43
1:E:1253:LEU:HA	1:E:1253:LEU:HD12	1.83	0.42
1:G:1228:ILE:HA	1:G:1229:PRO:HD3	1.81	0.42
1:H:1211:LEU:N	1:H:1211:LEU:HD12	2.34	0.42
1:B:1090:LEU:HD23	1:B:1090:LEU:HA	1.81	0.42
1:C:1114:VAL:HB	1:C:1157:ALA:HA	2.00	0.42
1:C:1163:TYR:CB	1:C:1164:PRO:CD	2.97	0.42
1:E:1072:PRO:HG2	1:F:1072:PRO:HD2	2.01	0.42
1:G:1163:TYR:HA	1:G:1168:ARG:HB2	2.00	0.42
1:A:1021:LEU:HD23	1:A:1021:LEU:C	2.39	0.42
1:C:1032:GLU:HG3	1:C:1053:TRP:CH2	2.55	0.42
1:C:1091:ARG:HG3	1:C:1092:ILE:N	2.34	0.42
1:H:1158:SER:HB2	1:H:1200:ALA:HB2	2.01	0.42
1:I:1140:LEU:HD12	1:I:1140:LEU:HA	1.82	0.42
1:A:1024:VAL:HA	1:A:1065:CYS:O	2.19	0.42
1:A:1089:PHE:O	1:A:1213:ALA:HA	2.19	0.42
1:E:1126:MET:SD	1:D:1127:GLU:HG3	2.60	0.42
1:F:1185:GLU:HG3	1:F:1186:GLU:N	2.29	0.42
1:F:1203:LEU:HD12	1:F:1203:LEU:HA	1.70	0.42
1:I:1175:ARG:HD2	6:I:1309:HOH:O	2.19	0.42
1:A:1024:VAL:O	1:A:1024:VAL:HG23	2.20	0.42
1:D:1060[A]:LYS:HD3	1:D:1061:ALA:H	1.83	0.42
1:G:1136:CYS:O	1:G:1140:LEU:HD13	2.20	0.42
1:G:1115:ARG:NE	1:G:1120:SER:OG	2.51	0.42
1:H:1030:ARG:O	1:H:1034:ILE:HG22	2.20	0.42
1:I:1007:PHE:HD2	1:I:1008:HIS:CE1	2.37	0.42
1:A:1235:LYS:HD3	1:A:1236:GLN:H	1.85	0.42
1:H:1108:LEU:CD2	1:H:1152:HIS:HB2	2.50	0.42
1:H:1238:GLU:HG3	1:H:1239:SER:N	2.34	0.42
1:E:1049:GLU:CG	1:F:1049:GLU:HG2	2.49	0.42
1:C:1126:MET:HG3	1:B:1126:MET:HG3	2.01	0.41
1:G:1009:LEU:HD11	1:G:1081:LEU:HG	2.02	0.41
1:I:1102:ILE:HD11	1:I:1219:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1003:LYS:HB3	1:C:1003:LYS:HE2	1.83	0.41
1:F:1178:ARG:HH21	1:D:1186:GLU:CD	2.22	0.41
1:G:1079:GLU:O	1:G:1083:GLN:HG3	2.19	0.41
1:I:1108:LEU:HD22	1:I:1152:HIS:HB2	2.01	0.41
1:H:1139:ALA:O	1:H:1143:ALA:N	2.46	0.41
1:A:1081:LEU:HD12	1:A:1081:LEU:HA	1.91	0.41
1:A:1144:ALA:CA	1:A:1244:ILE:HD12	2.48	0.41
1:F:1158:SER:CB	1:F:1200:ALA:HB2	2.46	0.41
1:F:1024:VAL:HA	1:F:1025:PRO:HD2	1.96	0.41
1:I:1157:ALA:HB2	1:I:1192:VAL:HG11	2.03	0.41
1:C:1092:ILE:O	1:C:1092:ILE:HG23	2.21	0.41
1:G:1050:PHE:HE2	1:G:1077:ALA:HB2	1.86	0.41
1:G:1153:VAL:O	1:G:1193:MET:HE1	2.20	0.41
1:I:1163:TYR:CB	1:I:1164:PRO:HD3	2.37	0.41
1:H:1228:ILE:HA	1:H:1229:PRO:HD3	1.92	0.40
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	2.02	0.40
1:A:1228:ILE:HA	1:A:1229:PRO:HD3	1.95	0.40
1:B:1024:VAL:O	1:B:1024:VAL:HG23	2.21	0.40
1:G:1144:ALA:HA	1:G:1244:ILE:HD12	2.03	0.40
1:G:1187:TRP:HB3	1:G:1192:VAL:HB	2.03	0.40
2:C:1301:URF:N1	3:C:1303:GOL:H2	2.35	0.40
1:D:1095:THR:OG1	1:D:1194:ASN:HB2	2.21	0.40
1:G:1009:LEU:CD1	1:G:1081:LEU:HG	2.52	0.40
1:H:1163:TYR:CB	1:H:1164:PRO:HD3	2.51	0.40
1:A:1079:GLU:OE1	1:B:1171:THR:HB	2.21	0.40
1:I:1056:GLU:HG2	1:I:1061:ALA:HA	2.02	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	245/253 (97%)	239 (98%)	5 (2%)	1 (0%)	38	32
1	B	241/253 (95%)	234 (97%)	6 (2%)	1 (0%)	38	32
1	C	242/253 (96%)	235 (97%)	5 (2%)	2 (1%)	22	14
1	D	242/253 (96%)	237 (98%)	4 (2%)	1 (0%)	38	32
1	E	241/253 (95%)	236 (98%)	4 (2%)	1 (0%)	38	32
1	F	238/253 (94%)	232 (98%)	5 (2%)	1 (0%)	38	32
1	G	238/253 (94%)	223 (94%)	14 (6%)	1 (0%)	38	32
1	H	239/253 (94%)	228 (95%)	9 (4%)	2 (1%)	22	14
1	I	239/253 (94%)	229 (96%)	9 (4%)	1 (0%)	38	32
All	All	2165/2277 (95%)	2093 (97%)	61 (3%)	11 (0%)	32	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1163	TYR
1	F	1163	TYR
1	D	1163	TYR
1	C	1163	TYR
1	A	1163	TYR
1	E	1163	TYR
1	B	1163	TYR
1	C	1231	ALA
1	H	1170	ASP
1	G	1163	TYR
1	I	1163	TYR

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	198/202 (98%)	192 (97%)	6 (3%)	46	45
1	B	195/202 (96%)	189 (97%)	6 (3%)	45	44
1	C	195/202 (96%)	189 (97%)	6 (3%)	45	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	195/202 (96%)	192 (98%)	3 (2%)	70	75
1	E	194/202 (96%)	187 (96%)	7 (4%)	40	38
1	F	192/202 (95%)	188 (98%)	4 (2%)	59	62
1	G	192/202 (95%)	181 (94%)	11 (6%)	24	18
1	H	193/202 (96%)	181 (94%)	12 (6%)	21	15
1	I	193/202 (96%)	185 (96%)	8 (4%)	35	33
All	All	1747/1818 (96%)	1684 (96%)	63 (4%)	40	38

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1081	LEU
1	A	1185	GLU
1	A	1196	GLU
1	A	1203	LEU
1	A	1235	LYS
1	A	1253	LEU
1	E	1029	GLU
1	E	1049	GLU
1	E	1185	GLU
1	E	1196	GLU
1	E	1203	LEU
1	E	1240	HIS
1	E	1253	LEU
1	F	1030	ARG
1	F	1185	GLU
1	F	1196	GLU
1	F	1203	LEU
1	D	1038	MET
1	D	1092	ILE
1	D	1196	GLU
1	C	1003	LYS
1	C	1037	LEU
1	C	1145	LYS
1	C	1196	GLU
1	C	1225	GLN
1	C	1253	LEU
1	B	1049	GLU
1	B	1196	GLU
1	B	1203	LEU

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Mol	Chain	Res	Type
1	B	1215	MET
1	B	1238	GLU
1	B	1240	HIS
1	H	1024	VAL
1	H	1033	LYS
1	H	1034	ILE
1	H	1044	LEU
1	H	1049	GLU
1	H	1052	SER
1	H	1060	LYS
1	H	1091	ARG
1	H	1175	ARG
1	H	1181	LYS
1	H	1196	GLU
1	H	1250	ARG
1	I	1049	GLU
1	I	1091	ARG
1	I	1102	ILE
1	I	1160	ASP
1	I	1185	GLU
1	I	1196	GLU
1	I	1203	LEU
1	I	1240	HIS
1	G	1034	ILE
1	G	1039	ASP
1	G	1043	LYS
1	G	1091	ARG
1	G	1092	ILE
1	G	1095	THR
1	G	1160	ASP
1	G	1196	GLU
1	G	1203	LEU
1	G	1216	VAL
1	G	1253	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1209	GLN

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 ⓘ

Of 17 ligands modelled in this entry, 3 are 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	URF	A	1301	-	8,9,9	3.94	4 (50%)	6,12,12	6.00	4 (66%)
3	GOL	A	1302	-	5,5,5	0.28	0	5,5,5	0.66	0
2	URF	B	1301	-	8,9,9	3.71	4 (50%)	6,12,12	5.72	4 (66%)
3	GOL	B	1302	-	5,5,5	0.35	0	5,5,5	0.16	0
2	URF	C	1301	-	8,9,9	4.02	4 (50%)	6,12,12	5.78	4 (66%)
5	EDO	C	1302	-	3,3,3	0.40	0	2,2,2	0.37	0
3	GOL	C	1303	-	5,5,5	0.33	0	5,5,5	0.19	0
2	URF	D	1301	-	8,9,9	3.95	4 (50%)	6,12,12	5.47	4 (66%)
2	URF	E	1301	-	8,9,9	3.62	4 (50%)	6,12,12	5.29	3 (50%)
3	GOL	E	1302	-	5,5,5	0.37	0	5,5,5	0.34	0
2	URF	F	1301	-	8,9,9	3.99	4 (50%)	6,12,12	5.63	4 (66%)
3	GOL	F	1302	-	5,5,5	0.33	0	5,5,5	0.43	0
2	URF	G	1301	-	8,9,9	4.01	5 (62%)	6,12,12	5.71	4 (66%)
2	URF	H	1301	-	8,9,9	4.03	5 (62%)	6,12,12	5.53	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	URF	A	1301	-	-	0/0/0/0	0/1/1/1
3	GOL	A	1302	-	-	0/4/4/4	0/0/0/0
2	URF	B	1301	-	-	0/0/0/0	0/1/1/1
3	GOL	B	1302	-	-	0/4/4/4	0/0/0/0
2	URF	C	1301	-	-	0/0/0/0	0/1/1/1
5	EDO	C	1302	-	-	0/1/1/1	0/0/0/0
3	GOL	C	1303	-	-	0/4/4/4	0/0/0/0
2	URF	D	1301	-	-	0/0/0/0	0/1/1/1
2	URF	E	1301	-	-	0/0/0/0	0/1/1/1
3	GOL	E	1302	-	-	0/4/4/4	0/0/0/0
2	URF	F	1301	-	-	0/0/0/0	0/1/1/1
3	GOL	F	1302	-	-	0/4/4/4	0/0/0/0
2	URF	G	1301	-	-	0/0/0/0	0/1/1/1
2	URF	H	1301	-	-	0/0/0/0	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1301	URF	C2-N3	2.02	1.42	1.38
2	H	1301	URF	C2-N3	2.10	1.42	1.38
2	E	1301	URF	C2-N1	2.61	1.43	1.38
2	F	1301	URF	C2-N1	2.75	1.43	1.38
2	B	1301	URF	C2-N1	2.77	1.43	1.38
2	H	1301	URF	C2-N1	2.87	1.43	1.38
2	G	1301	URF	C2-N1	3.00	1.44	1.38
2	C	1301	URF	C2-N1	3.00	1.44	1.38
2	A	1301	URF	C2-N1	3.08	1.44	1.38
2	D	1301	URF	C2-N1	3.34	1.44	1.38
2	E	1301	URF	C4-N3	3.70	1.39	1.33
2	C	1301	URF	C4-N3	4.12	1.40	1.33
2	A	1301	URF	C4-N3	4.23	1.40	1.33
2	B	1301	URF	C4-N3	4.24	1.40	1.33
2	D	1301	URF	C4-N3	4.29	1.40	1.33
2	F	1301	URF	C4-N3	4.30	1.40	1.33
2	B	1301	URF	C6-N1	4.52	1.44	1.34
2	G	1301	URF	C4-N3	4.55	1.41	1.33
2	H	1301	URF	C4-N3	4.62	1.41	1.33
2	D	1301	URF	C6-N1	4.88	1.44	1.34
2	C	1301	URF	C6-N1	5.00	1.45	1.34
2	A	1301	URF	C6-N1	5.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1301	URF	C6-N1	5.03	1.45	1.34
2	E	1301	URF	C6-N1	5.03	1.45	1.34
2	H	1301	URF	C6-N1	5.05	1.45	1.34
2	G	1301	URF	C6-N1	5.10	1.45	1.34
2	E	1301	URF	C4-C5	7.19	1.47	1.38
2	B	1301	URF	C4-C5	7.65	1.47	1.38
2	D	1301	URF	C4-C5	8.00	1.48	1.38
2	A	1301	URF	C4-C5	8.08	1.48	1.38
2	G	1301	URF	C4-C5	8.11	1.48	1.38
2	H	1301	URF	C4-C5	8.22	1.48	1.38
2	F	1301	URF	C4-C5	8.30	1.48	1.38
2	C	1301	URF	C4-C5	8.52	1.49	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	URF	N1-C2-N3	-12.43	119.46	128.40
2	B	1301	URF	N1-C2-N3	-12.26	119.58	128.40
2	C	1301	URF	N1-C2-N3	-11.99	119.78	128.40
2	G	1301	URF	N1-C2-N3	-11.95	119.81	128.40
2	F	1301	URF	N1-C2-N3	-11.78	119.92	128.40
2	H	1301	URF	N1-C2-N3	-11.57	120.08	128.40
2	E	1301	URF	N1-C2-N3	-11.46	120.16	128.40
2	D	1301	URF	N1-C2-N3	-11.36	120.23	128.40
2	A	1301	URF	C5-C4-N3	-3.01	119.22	122.39
2	D	1301	URF	C5-C4-N3	-2.89	119.34	122.39
2	C	1301	URF	C5-C4-N3	-2.84	119.39	122.39
2	H	1301	URF	C5-C4-N3	-2.72	119.52	122.39
2	F	1301	URF	C5-C4-N3	-2.68	119.56	122.39
2	G	1301	URF	C5-C4-N3	-2.63	119.62	122.39
2	B	1301	URF	C5-C4-N3	-2.29	119.98	122.39
2	D	1301	URF	C6-N1-C2	2.76	119.78	115.36
2	H	1301	URF	C6-N1-C2	2.84	119.90	115.36
2	G	1301	URF	C6-N1-C2	2.93	120.05	115.36
2	F	1301	URF	C6-N1-C2	3.11	120.34	115.36
2	A	1301	URF	C6-N1-C2	3.13	120.37	115.36
2	C	1301	URF	C6-N1-C2	3.15	120.40	115.36
2	E	1301	URF	C6-N1-C2	3.31	120.65	115.36
2	B	1301	URF	C6-N1-C2	3.51	120.97	115.36
2	E	1301	URF	C4-N3-C2	4.70	119.27	115.16
2	B	1301	URF	C4-N3-C2	5.29	119.78	115.16
2	H	1301	URF	C4-N3-C2	5.77	120.20	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1301	URF	C4-N3-C2	5.78	120.22	115.16
2	D	1301	URF	C4-N3-C2	5.78	120.22	115.16
2	G	1301	URF	C4-N3-C2	6.04	120.44	115.16
2	C	1301	URF	C4-N3-C2	6.16	120.55	115.16
2	A	1301	URF	C4-N3-C2	6.48	120.83	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	URF	1	0
3	A	1302	GOL	1	0
2	B	1301	URF	2	0
3	B	1302	GOL	3	0
2	C	1301	URF	2	0
5	C	1302	EDO	4	0
3	C	1303	GOL	2	0
2	E	1301	URF	1	0
3	E	1302	GOL	2	0
2	F	1301	URF	1	0
3	F	1302	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/253 (98%)	0.02	11 (4%) 35 43	26, 39, 62, 113	0
1	B	244/253 (96%)	-0.09	3 (1%) 79 83	27, 41, 64, 102	0
1	C	246/253 (97%)	0.10	9 (3%) 42 48	25, 39, 61, 107	0
1	D	245/253 (96%)	0.04	12 (4%) 30 38	23, 38, 62, 96	0
1	E	245/253 (96%)	-0.12	6 (2%) 59 67	26, 39, 60, 114	0
1	F	242/253 (95%)	-0.12	3 (1%) 79 83	26, 39, 57, 78	0
1	G	242/253 (95%)	1.55	84 (34%) 0 1	57, 89, 119, 135	0
1	H	243/253 (96%)	0.80	39 (16%) 2 3	45, 72, 104, 128	0
1	I	243/253 (96%)	1.38	71 (29%) 1 1	39, 77, 121, 130	0
All	All	2198/2277 (96%)	0.40	238 (10%) 6 9	23, 47, 108, 135	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1231	ALA	9.1
1	G	1148	GLY	8.3
1	C	1231	ALA	7.9
1	G	1252	LEU	7.7
1	I	1146	SER	7.3
1	I	1029	GLU	7.0
1	I	1016	LEU	6.4
1	I	1003	LYS	6.4
1	G	1147	ILE	6.3
1	A	1236	GLN	6.3
1	E	1237	THR	6.3
1	D	1231	ALA	6.2
1	D	1003	LYS	6.1
1	H	1238	GLU	6.0
1	I	1253	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	I	1053	TRP	5.9
1	E	1231	ALA	5.8
1	H	1053	TRP	5.7
1	I	1147	ILE	5.7
1	I	1092	ILE	5.6
1	A	1237	THR	5.5
1	I	1058	ASP	5.5
1	G	1014	ASN	5.4
1	G	1230	ASN	5.2
1	I	1017	GLN	5.2
1	G	1024	VAL	5.0
1	G	1026	GLY	5.0
1	I	1225	GLN	5.0
1	G	1143	ALA	5.0
1	B	1003	LYS	4.9
1	G	1146	SER	4.9
1	H	1011	LEU	4.7
1	I	1024	VAL	4.6
1	G	1029	GLU	4.6
1	H	1244	ILE	4.5
1	I	1044	LEU	4.4
1	E	1239	SER	4.4
1	I	1043	LYS	4.4
1	I	1103	ASN	4.3
1	C	1232	GLU	4.2
1	G	1010	GLY	4.2
1	A	1003	LYS	4.2
1	D	1253	LEU	4.1
1	H	1250	ARG	4.0
1	I	1036	ALA	4.0
1	G	1239	SER	3.9
1	G	1034	ILE	3.9
1	G	1107	VAL	3.9
1	I	1046	SER	3.8
1	G	1053	TRP	3.8
1	I	1026	GLY	3.8
1	G	1253	LEU	3.7
1	G	1036	ALA	3.7
1	F	1230	ASN	3.7
1	C	1238	GLU	3.7
1	G	1025	PRO	3.7
1	G	1057	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	1232	GLU	3.7
1	G	1245	VAL	3.7
1	H	1149	ALA	3.7
1	G	1092	ILE	3.6
1	I	1149	ALA	3.6
1	C	1253	LEU	3.6
1	G	1145	LYS	3.6
1	I	1023	ILE	3.6
1	A	1238	GLU	3.6
1	H	1057	LEU	3.6
1	I	1038	MET	3.6
1	G	1056	GLU	3.5
1	G	1104	VAL	3.5
1	G	1195	TYR	3.5
1	G	1012	THR	3.5
1	I	1025	PRO	3.5
1	G	1058	ASP	3.5
1	I	1145	LYS	3.5
1	G	1137	THR	3.4
1	A	1230	ASN	3.4
1	G	1032	GLU	3.4
1	H	1038	MET	3.4
1	G	1061	ALA	3.4
1	H	1253	LEU	3.4
1	H	1237	THR	3.4
1	A	1235	LYS	3.4
1	E	1238	GLU	3.3
1	I	1060	LYS	3.3
1	H	1146	SER	3.3
1	H	1230	ASN	3.2
1	G	1067	THR	3.2
1	G	1136	CYS	3.2
1	H	1069	ILE	3.2
1	I	1144	ALA	3.1
1	G	1005	ASP	3.1
1	I	1252	LEU	3.1
1	I	1018	GLY	3.1
1	G	1140	LEU	3.1
1	H	1055	ALA	3.1
1	G	1019	ALA	3.1
1	I	1073	SER	3.1
1	C	1202	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	1036	ALA	3.0
1	G	1063	ILE	3.0
1	I	1247	GLU	3.0
1	G	1041	PRO	3.0
1	I	1012	THR	3.0
1	C	1003	LYS	3.0
1	I	1246	VAL	3.0
1	G	1215	MET	3.0
1	G	1015	ASP	3.0
1	H	1035	ALA	3.0
1	I	1091	ARG	2.9
1	G	1038	MET	2.9
1	I	1230	ASN	2.9
1	G	1091	ARG	2.9
1	E	1230	ASN	2.9
1	A	1004	SER	2.9
1	G	1211	LEU	2.8
1	G	1221	VAL	2.8
1	G	1241	ALA	2.8
1	I	1250	ARG	2.8
1	G	1229	PRO	2.8
1	H	1042	VAL	2.7
1	G	1226	GLN	2.7
1	I	1052	SER	2.7
1	G	1098	ILE	2.7
1	G	1154	GLY	2.7
1	G	1227	GLU	2.7
1	H	1251	ARG	2.7
1	G	1022	ALA	2.7
1	G	1248	ALA	2.7
1	I	1090	LEU	2.7
1	G	1023	ILE	2.7
1	I	1148	GLY	2.7
1	H	1148	GLY	2.6
1	I	1059	GLY	2.6
1	I	1013	LYS	2.6
1	I	1202	LEU	2.6
1	H	1039	ASP	2.6
1	G	1216	VAL	2.6
1	I	1041	PRO	2.6
1	G	1016	LEU	2.6
1	H	1172	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	1067	THR	2.5
1	I	1040	LYS	2.5
1	I	1054	ARG	2.5
1	G	1134	PHE	2.5
1	G	1144	ALA	2.5
1	I	1005	ASP	2.5
1	I	1102	ILE	2.5
1	G	1069	ILE	2.5
1	I	1042	VAL	2.5
1	G	1033	LYS	2.5
1	I	1047	HIS	2.4
1	G	1011	LEU	2.4
1	I	1243	LYS	2.4
1	D	1091	ARG	2.4
1	G	1217	ALA	2.4
1	H	1243	LYS	2.4
1	G	1224	THR	2.4
1	I	1056	GLU	2.4
1	I	1251	ARG	2.4
1	H	1074	THR	2.4
1	I	1004	SER	2.4
1	D	1024	VAL	2.4
1	H	1248	ALA	2.4
1	I	1022	ALA	2.4
1	I	1068	GLY	2.4
1	G	1059	GLY	2.4
1	G	1093	GLY	2.4
1	G	1214	GLY	2.4
1	G	1108	LEU	2.3
1	I	1216	VAL	2.3
1	H	1073	SER	2.3
1	H	1070	GLY	2.3
1	I	1037	LEU	2.3
1	I	1188	GLN	2.3
1	G	1040	LYS	2.3
1	C	1216	VAL	2.3
1	I	1074	THR	2.3
1	G	1102	ILE	2.3
1	C	1090	LEU	2.3
1	G	1132	ALA	2.3
1	I	1051	THR	2.3
1	A	1069	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1092	ILE	2.3
1	H	1033	LYS	2.3
1	D	1239	SER	2.3
1	I	1198	GLU	2.3
1	G	1086	ILE	2.3
1	G	1084	LEU	2.2
1	I	1240	HIS	2.2
1	G	1240	HIS	2.2
1	G	1004	SER	2.2
1	I	1185	GLU	2.2
1	D	1250	ARG	2.2
1	D	1092	ILE	2.2
1	H	1032	GLU	2.2
1	I	1032	GLU	2.2
1	E	1104	VAL	2.2
1	G	1242	VAL	2.2
1	I	1011	LEU	2.2
1	G	1050	PHE	2.2
1	I	1069	ILE	2.2
1	G	1071	GLY	2.2
1	H	1072	PRO	2.2
1	G	1042	VAL	2.2
1	H	1199	SER	2.2
1	H	1034	ILE	2.1
1	G	1047	HIS	2.1
1	A	1093	GLY	2.1
1	D	1225	GLN	2.1
1	H	1239	SER	2.1
1	F	1145	LYS	2.1
1	I	1101	HIS	2.1
1	H	1106	ASP	2.1
1	G	1065	CYS	2.1
1	F	1239	SER	2.1
1	B	1230	ASN	2.1
1	I	1033	LYS	2.1
1	H	1058	ASP	2.1
1	G	1090	LEU	2.1
1	H	1240	HIS	2.1
1	I	1015	ASP	2.1
1	H	1068	GLY	2.1
1	G	1096	GLY	2.1
1	H	1076	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	1034	ILE	2.1
1	G	1068	GLY	2.1
1	D	1004	SER	2.0
1	I	1229	PRO	2.0
1	H	1047	HIS	2.0
1	I	1077	ALA	2.0
1	G	1243	LYS	2.0
1	A	1225	GLN	2.0
1	G	1064	VAL	2.0
1	B	1004	SER	2.0
1	D	1202	LEU	2.0
1	G	1051	THR	2.0
1	H	1145	LYS	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
4	K	D	1302	1/1	0.01	0.49	17.71	104,104,104,104	0
3	GOL	F	1302	6/6	0.75	0.48	11.77	61,65,66,66	0
3	GOL	C	1303	6/6	0.77	0.31	5.59	66,70,70,71	0
3	GOL	B	1302	6/6	0.89	0.26	3.27	55,56,58,58	0
3	GOL	E	1302	6/6	0.90	0.25	3.01	60,63,64,64	0
3	GOL	A	1302	6/6	0.78	0.31	2.45	66,68,68,69	0
2	URF	H	1301	9/9	0.84	0.18	1.54	71,72,73,73	0
2	URF	C	1301	9/9	0.93	0.14	1.40	33,37,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	URF	B	1301	9/9	0.93	0.13	1.31	30,31,36,37	0
2	URF	D	1301	9/9	0.92	0.12	0.76	32,33,35,38	0
2	URF	F	1301	9/9	0.94	0.14	0.72	43,44,46,47	0
2	URF	A	1301	9/9	0.92	0.13	0.30	38,40,42,43	0
2	URF	E	1301	9/9	0.96	0.11	0.04	25,26,31,32	0
4	K	A	1303	1/1	0.78	0.16	-0.61	61,61,61,61	0
2	URF	G	1301	9/9	0.90	0.18	-1.01	72,73,73,73	0
4	K	E	1303	1/1	0.81	0.14	-1.21	50,50,50,50	0
5	EDO	C	1302	4/4	0.88	0.27	-	43,43,45,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.