



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:39 PM GMT

PDB ID : 1Y1S  
Title : Crystal Structure of the Uridine Phosphorylase from Salmonella Typhimurium  
in Complex with Uracil and Sulfate Ion at 2.55Å Resolution  
Authors : Gabdoulkhakov, A.G.; Dontsova, M.V.; Kachalova, G.S.; Betzel, C.; Ealick,  
S.E.; Mikhailov, A.M.  
Deposited on : 2004-11-19  
Resolution : 2.55 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

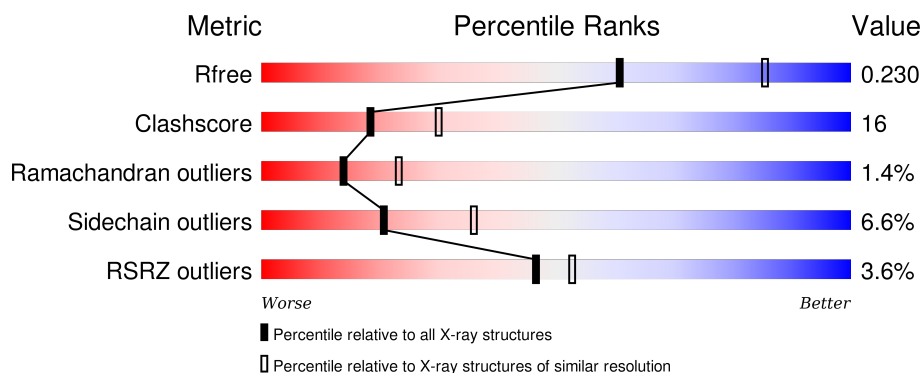
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>2%</div> <div>69% 26% ..</div> </div>
1	B	253	<div> <div>3%</div> <div>72% 23% ...</div> </div>
1	C	253	<div> <div>6%</div> <div>65% 30% ..</div> </div>
1	D	253	<div> <div>4%</div> <div>67% 27% ..</div> </div>
1	E	253	<div> <div>4%</div> <div>66% 28% 5% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	253	<div><div></div><div>3%</div><div>71%</div><div>25%</div><div>• •</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11544 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.

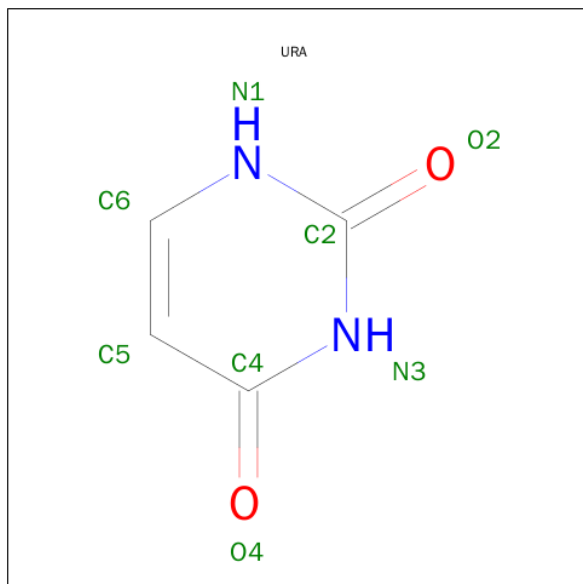
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	C	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	D	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	F	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	E	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	B	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is URACIL (three-letter code: URA) (formula:  $C_4H_4N_2O_2$ ).



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

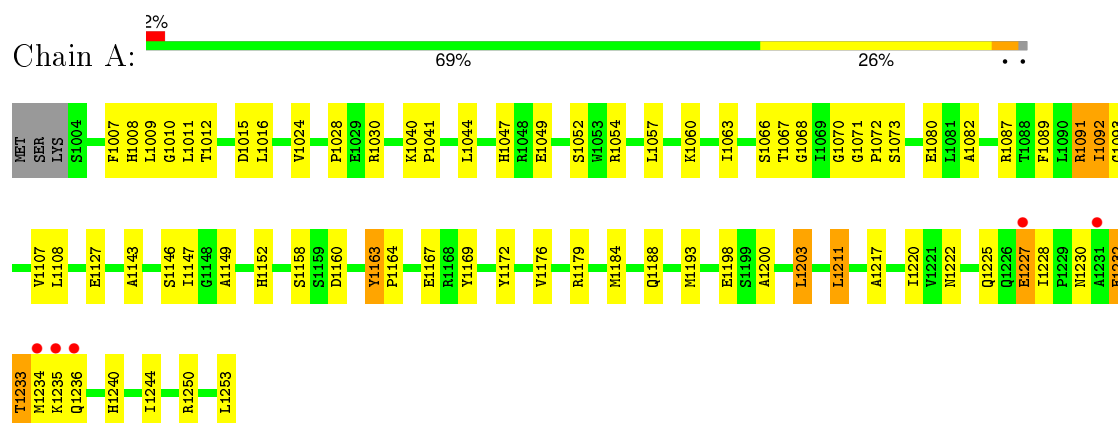
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	37	Total 37	O 37	0	0
4	C	33	Total 33	O 33	0	0
4	D	45	Total 45	O 45	0	0
4	E	25	Total 25	O 25	0	0
4	F	34	Total 34	O 34	0	0

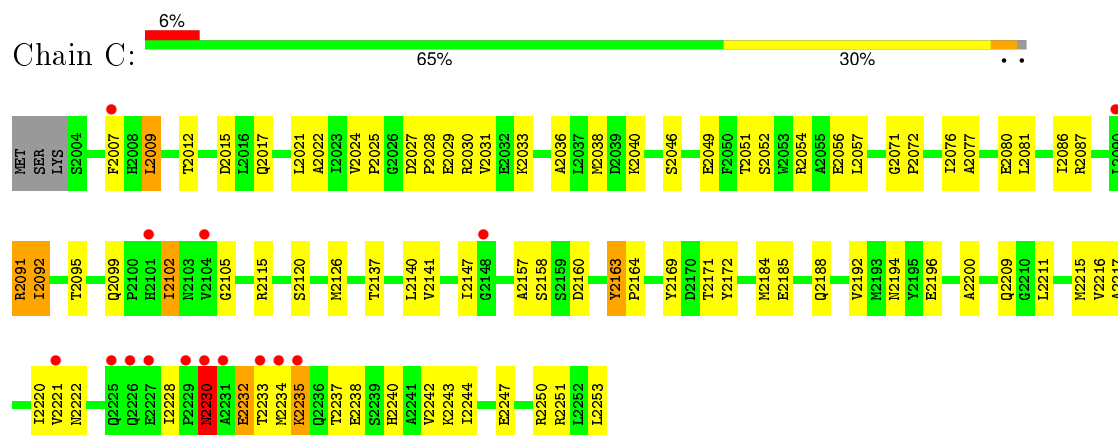
### 3 Residue-property plots

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

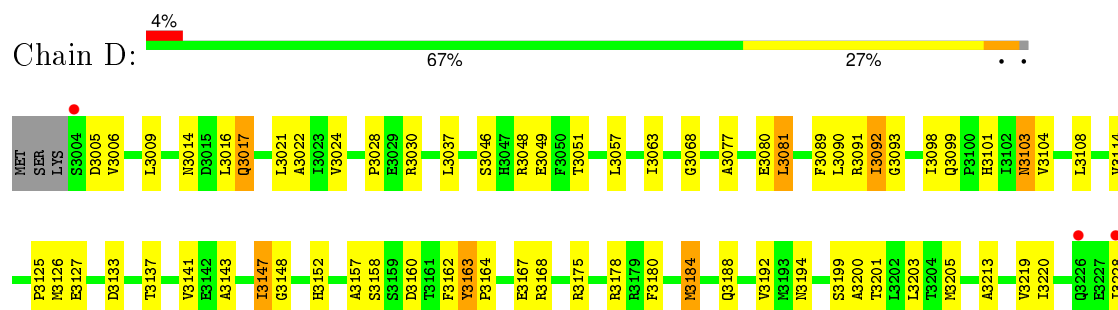
#### • Molecule 1: Uridine phosphorylase



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#### • Molecule 1: Uridine phosphorylase

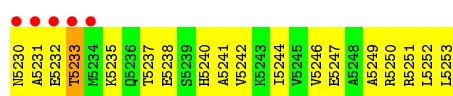




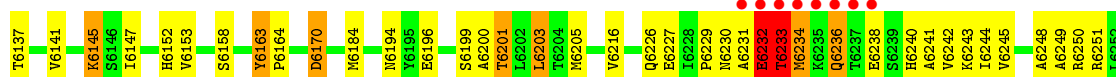
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.99Å 124.12Å 133.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.84 – 2.55 28.96 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.3 (26.84-2.55) 96.6 (28.96-2.51)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.92 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.231 0.189 , 0.230	Depositor DCC
$R_{free}$ test set	2357 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 49446 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: URA, SO4

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	0.35	0/1906	0.63	0/2584
1	B	0.40	1/1906 (0.1%)	0.75	5/2584 (0.2%)
1	C	0.35	0/1906	0.65	0/2584
1	D	0.34	0/1906	0.63	0/2584
1	E	0.39	0/1906	0.70	0/2584
1	F	0.38	0/1906	0.74	2/2584 (0.1%)
All	All	0.37	1/11436 (0.0%)	0.68	7/15504 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6232	GLU	CG-CD	5.33	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4231	ALA	N-CA-C	9.75	137.32	111.00
1	B	6231	ALA	N-CA-C	7.89	132.30	111.00
1	F	4230	ASN	N-CA-C	6.91	129.67	111.00
1	B	6233	THR	N-CA-C	6.42	128.33	111.00
1	B	6232	GLU	CA-C-N	-6.17	103.62	117.20
1	B	6232	GLU	N-CA-C	6.10	127.48	111.00
1	B	6232	GLU	C-N-CA	5.72	136.00	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	0	1887	51	0
1	B	1876	0	1887	50	0
1	C	1876	0	1887	72	0
1	D	1876	0	1887	62	0
1	E	1876	0	1887	66	0
1	F	1876	0	1887	62	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	8	0	3	0	0
3	B	8	0	3	0	0
3	D	8	0	3	0	0
3	E	8	0	3	0	0
3	F	8	0	3	0	0
4	A	44	0	0	1	0
4	B	37	0	0	4	0
4	C	33	0	0	0	0
4	D	45	0	0	0	0
4	E	25	0	0	2	0
4	F	34	0	0	2	0
All	All	11544	0	11337	352	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 16.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2235:LYS:HD2	1:C:2235:LYS:H	1.10	1.13
1:B:6232:GLU:OE1	1:B:6232:GLU:HA	1.65	0.95
1:B:6071:GLY:HA3	1:B:6201:THR:HG21	1.50	0.94
1:C:2235:LYS:N	1:C:2235:LYS:HD2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6201:THR:HG22	4:B:9210:HOH:O	1.72	0.90
1:E:5222:ASN:OD1	1:E:5224:THR:HG23	1.72	0.88
1:C:2091:ARG:HB3	1:C:2215:MET:HG3	1.58	0.85
1:C:2158:SER:HB3	1:C:2200:ALA:HB2	1.59	0.85
1:C:2099:GLN:HB2	1:C:2102:ILE:HG13	1.60	0.83
1:A:1091:ARG:HD3	4:A:9003:HOH:O	1.77	0.83
1:D:3236:GLN:HA	1:D:3236:GLN:HE21	1.42	0.82
1:E:5091:ARG:HG2	1:E:5215:MET:HG3	1.62	0.80
1:E:5163:TYR:HB2	1:E:5164:PRO:HD3	1.63	0.79
1:E:5158:SER:HB3	1:E:5200:ALA:HB2	1.63	0.79
1:D:3229:PRO:CA	1:D:3233:THR:HG21	2.12	0.78
1:B:6158:SER:HB3	1:B:6200:ALA:HB2	1.64	0.78
1:B:6057:LEU:HG	1:B:6250:ARG:HG2	1.67	0.77
1:C:2232:GLU:OE1	1:C:2235:LYS:HB2	1.86	0.76
1:D:3233:THR:HG23	1:D:3234:MET:H	1.51	0.76
1:C:2081:LEU:HD22	1:C:2086:ILE:HG13	1.68	0.76
1:B:6071:GLY:CA	1:B:6201:THR:HG21	2.17	0.74
1:F:4235:LYS:HG2	1:F:4236:GLN:HE21	1.52	0.74
1:C:2040:LYS:HD2	1:C:2040:LYS:N	2.02	0.74
1:A:1220:ILE:HB	1:A:1233:THR:HG23	1.70	0.74
1:B:6242:VAL:O	1:B:6245:VAL:HG12	1.89	0.73
1:D:3229:PRO:HA	1:D:3233:THR:HG21	1.69	0.73
1:F:4086:ILE:C	1:F:4087:ARG:HD2	2.10	0.72
1:E:5249:ALA:O	1:E:5253:LEU:HD13	1.89	0.72
1:F:4185:GLU:HG2	4:F:9048:HOH:O	1.89	0.72
1:A:1232:GLU:HA	1:A:1235:LYS:HB3	1.73	0.71
1:F:4092:ILE:HD11	1:F:4241:ALA:HB1	1.70	0.71
1:B:6137:THR:O	1:B:6141:VAL:HG23	1.91	0.71
1:D:3030:ARG:HH12	1:D:3093:GLY:HA2	1.54	0.70
1:C:2076:ILE:O	1:C:2080:GLU:HG3	1.92	0.70
1:B:6031:VAL:HG21	1:B:6051:THR:O	1.91	0.70
1:D:3220:ILE:HB	1:D:3234:MET:HG2	1.74	0.69
1:F:4030:ARG:HA	1:F:4033:LYS:HD3	1.75	0.69
1:A:1049:GLU:HB3	1:F:4049:GLU:HB3	1.75	0.69
1:B:6216:VAL:HG21	1:B:6244:ILE:HD11	1.75	0.68
1:D:3228:ILE:HD12	1:D:3228:ILE:N	2.08	0.68
1:C:2009:LEU:HD22	1:C:2080:GLU:HB2	1.76	0.68
1:D:3228:ILE:HG22	1:D:3229:PRO:HD2	1.76	0.67
1:B:6029:GLU:O	1:B:6029:GLU:HG2	1.96	0.65
1:F:4158:SER:HB3	1:F:4200:ALA:HB2	1.77	0.65
1:E:5091:ARG:HG2	1:E:5215:MET:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4092:ILE:HD11	1:F:4241:ALA:CB	2.26	0.65
1:E:5031:VAL:HG13	1:E:5064:VAL:HG12	1.80	0.64
1:A:1184:MET:O	1:A:1188:GLN:HG3	1.96	0.64
1:B:6226:GLN:NE2	1:B:6229:PRO:HA	2.13	0.64
1:E:5227:GLU:OE1	1:E:5227:GLU:HA	1.97	0.64
1:D:3184:MET:O	1:D:3188:GLN:HG3	1.98	0.63
1:E:5030:ARG:HD3	1:E:5238:GLU:OE1	1.99	0.63
1:B:6240:HIS:O	1:B:6244:ILE:HG23	1.98	0.63
1:B:6232:GLU:OE1	1:B:6233:THR:HG22	1.98	0.62
1:A:1172:TYR:HE2	1:F:4087:ARG:HH21	1.47	0.62
1:F:4242:VAL:O	1:F:4246:VAL:HG23	1.97	0.62
1:D:3163:TYR:HA	1:D:3168:ARG:HD2	1.82	0.62
1:C:2105:GLY:HA2	1:C:2237:THR:CG2	2.30	0.62
1:F:4235:LYS:HG2	1:F:4236:GLN:NE2	2.15	0.61
1:F:4030:ARG:HH11	1:F:4033:LYS:HE3	1.65	0.61
1:C:2140:LEU:HD22	1:C:2216:VAL:HB	1.81	0.61
1:B:6021:LEU:HD23	1:B:6022:ALA:N	2.15	0.61
1:E:5114:VAL:HG12	1:E:5116:LEU:HD13	1.83	0.60
1:B:6243:LYS:HD3	1:B:6243:LYS:C	2.21	0.60
1:A:1222:ASN:HB3	1:A:1225:GLN:HE21	1.65	0.60
1:D:3233:THR:HG23	1:D:3234:MET:N	2.16	0.60
1:D:3104:VAL:HA	1:D:3219:VAL:HG12	1.82	0.60
1:C:2220:ILE:HG13	1:C:2221:VAL:N	2.17	0.60
1:B:6009:LEU:CD1	1:B:6081:LEU:HD13	2.31	0.60
1:E:5142:GLU:O	1:E:5145:LYS:HG2	2.01	0.60
1:A:1172:TYR:HE2	1:F:4087:ARG:NH2	1.99	0.60
1:B:6049:GLU:HG3	1:B:6068:GLY:HA3	1.84	0.60
1:B:6021:LEU:HD23	1:B:6021:LEU:C	2.23	0.59
1:B:6009:LEU:HD13	1:B:6081:LEU:HD13	1.84	0.59
1:F:4110:THR:HG23	1:F:4156:THR:HG23	1.82	0.59
1:C:2220:ILE:HG13	1:C:2221:VAL:H	1.67	0.59
1:F:4235:LYS:HB2	1:F:4235:LYS:NZ	2.18	0.59
1:E:5089:PHE:O	1:E:5213:ALA:HA	2.03	0.59
1:B:6104:VAL:HG13	4:B:9016:HOH:O	2.02	0.59
1:C:2240:HIS:O	1:C:2244:ILE:HG13	2.02	0.59
1:E:5240:HIS:O	1:E:5244:ILE:HG13	2.03	0.59
1:A:1227:GLU:O	1:A:1228:ILE:HD13	2.02	0.59
1:C:2230:ASN:ND2	1:C:2232:GLU:O	2.35	0.58
1:D:3049:GLU:HB3	1:B:6049:GLU:HB3	1.85	0.58
1:B:6077:ALA:O	1:B:6081:LEU:HB2	2.04	0.58
1:C:2147:ILE:HG22	1:C:2147:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:THR:HG22	1:A:1015:ASP:OD2	2.04	0.58
1:A:1011:LEU:HD21	1:A:1052:SER:OG	2.04	0.58
1:D:3021:LEU:HD23	1:D:3021:LEU:C	2.25	0.57
1:B:6056:GLU:CG	4:B:9195:HOH:O	2.50	0.57
1:A:1108:LEU:HD22	1:A:1152:HIS:HB2	1.85	0.57
1:C:2235:LYS:N	1:C:2235:LYS:CD	2.62	0.57
1:F:4087:ARG:N	1:F:4087:ARG:HD2	2.19	0.57
1:E:5092:ILE:HD13	1:E:5093:GLY:N	2.19	0.56
1:E:5230:ASN:O	1:E:5232:GLU:N	2.38	0.56
1:D:3228:ILE:CG2	1:D:3229:PRO:HD2	2.35	0.56
1:D:3230:ASN:OD1	1:D:3233:THR:HB	2.06	0.56
1:F:4233:THR:HB	1:F:4234:MET:SD	2.46	0.56
1:B:6056:GLU:HG3	4:B:9195:HOH:O	2.04	0.56
1:E:5138:THR:O	1:E:5142:GLU:HB2	2.06	0.55
1:F:4067:THR:HB	1:F:4074:THR:HA	1.88	0.55
1:B:6016:LEU:HD13	1:B:6086:ILE:CD1	2.36	0.55
1:E:5230:ASN:O	1:E:5233:THR:OG1	2.25	0.55
1:C:2095:THR:HG21	1:C:2194:ASN:ND2	2.21	0.55
1:F:4092:ILE:CD1	1:F:4241:ALA:HB1	2.36	0.55
1:D:3162:PHE:O	1:D:3168:ARG:HD2	2.08	0.54
1:F:4031:VAL:HG13	1:F:4064:VAL:HG12	1.88	0.54
1:B:6232:GLU:OE1	1:B:6232:GLU:CA	2.42	0.54
1:D:3098:ILE:HD11	1:D:3192:VAL:O	2.08	0.54
1:F:4098:ILE:HD11	1:F:4195:TYR:CE2	2.42	0.54
1:F:4021:LEU:C	1:F:4021:LEU:HD23	2.28	0.54
1:C:2209:GLN:HG2	1:E:5173:SER:HB3	1.89	0.54
1:C:2007:PHE:O	1:C:2007:PHE:CD2	2.61	0.54
1:E:5242:VAL:O	1:E:5246:VAL:HG23	2.08	0.54
1:C:2232:GLU:HB2	1:C:2235:LYS:HD3	1.90	0.54
1:E:5057:LEU:HB3	1:E:5253:LEU:HD21	1.90	0.54
1:C:2105:GLY:HA2	1:C:2237:THR:HG21	1.88	0.54
1:A:1143:ALA:O	1:A:1147:ILE:HG12	2.09	0.53
1:D:3163:TYR:HB2	1:D:3164:PRO:CD	2.38	0.53
1:B:6025:PRO:O	1:B:6066:SER:HA	2.09	0.53
1:A:1007:PHE:HD2	1:A:1008:HIS:CE1	2.27	0.53
1:E:5101:HIS:H	1:E:5101:HIS:CD2	2.26	0.53
1:F:4030:ARG:HG3	1:F:4238:GLU:OE2	2.09	0.53
1:F:4110:THR:HB	1:F:4215:MET:HB3	1.90	0.53
1:C:2021:LEU:C	1:C:2021:LEU:HD23	2.28	0.52
1:A:1163:TYR:HB2	1:A:1164:PRO:CD	2.38	0.52
1:A:1235:LYS:HG3	1:A:1236:GLN:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6115:ARG:NH2	1:B:6121:LEU:HD23	2.24	0.52
1:D:3092:ILE:C	1:D:3092:ILE:HD13	2.30	0.52
1:F:4238:GLU:O	1:F:4242:VAL:HG23	2.10	0.52
1:D:3099:GLN:HB3	1:D:3101:HIS:CE1	2.44	0.52
1:D:3238:GLU:O	1:D:3242:VAL:HG23	2.09	0.52
1:F:4150:THR:HG21	4:F:9108:HOH:O	2.09	0.52
1:E:5199:SER:O	1:E:5203:LEU:HB2	2.09	0.52
1:C:2028:PRO:HB3	1:C:2051:THR:CG2	2.40	0.51
1:D:3114:VAL:HB	1:D:3157:ALA:HA	1.91	0.51
1:E:5090:LEU:HD11	1:E:5252:LEU:HD12	1.93	0.51
1:A:1158:SER:HB3	1:A:1200:ALA:HB2	1.92	0.51
1:C:2046:SER:OG	1:C:2051:THR:HG22	2.10	0.51
1:D:3143:ALA:O	1:D:3147:ILE:HG22	2.09	0.51
1:A:1067:THR:O	1:A:1073:SER:HB3	2.09	0.51
1:B:6016:LEU:HD11	1:B:6084:LEU:HB3	1.93	0.51
1:F:4110:THR:OG1	1:F:4156:THR:HG21	2.10	0.51
1:C:2091:ARG:CB	1:C:2215:MET:HG3	2.33	0.51
1:D:3147:ILE:HD12	1:D:3147:ILE:O	2.11	0.51
1:B:6234:MET:SD	1:B:6234:MET:N	2.84	0.51
1:A:1149:ALA:HB2	1:A:1240:HIS:NE2	2.26	0.51
1:E:5163:TYR:CB	1:E:5164:PRO:HD3	2.38	0.51
1:A:1030:ARG:HH12	1:A:1093:GLY:HA2	1.75	0.51
1:D:3167:GLU:HG3	1:D:3180:PHE:O	2.11	0.51
1:B:6119:ALA:HB3	1:B:6201:THR:HB	1.92	0.51
1:F:4024:VAL:O	1:F:4024:VAL:HG23	2.11	0.51
1:A:1009:LEU:HD22	1:A:1080:GLU:HB2	1.93	0.51
1:B:6092:ILE:HD13	1:B:6092:ILE:C	2.30	0.50
1:E:5201:THR:O	1:E:5205:MET:HG2	2.11	0.50
1:A:1232:GLU:OE2	1:A:1232:GLU:HA	2.12	0.50
1:C:2147:ILE:HG21	1:C:2243:LYS:HE3	1.93	0.50
1:E:5006:VAL:HG21	1:E:5009:LEU:HB2	1.93	0.50
1:D:3158:SER:HB3	1:D:3200:ALA:HB2	1.92	0.50
1:A:1092:ILE:C	1:A:1092:ILE:HD13	2.31	0.50
1:D:3103:ASN:ND2	1:D:3103:ASN:H	2.07	0.50
1:A:1044:LEU:HD11	1:A:1054:ARG:HB2	1.93	0.50
1:E:5057:LEU:HD11	1:E:5250:ARG:NH2	2.27	0.50
1:B:6147:ILE:CD1	1:B:6243:LYS:HD2	2.41	0.50
1:D:3098:ILE:HD13	1:D:3188:GLN:HG2	1.94	0.50
1:B:6170:ASP:HB2	1:B:6227:GLU:OE2	2.11	0.50
1:A:1040:LYS:N	1:A:1041:PRO:HD3	2.27	0.50
1:A:1028:PRO:HA	1:A:1066:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4059:GLY:O	1:F:4060:LYS:HD2	2.12	0.50
1:C:2115:ARG:NE	1:C:2120:SER:HB3	2.27	0.49
1:D:3092:ILE:O	1:D:3092:ILE:HG23	2.12	0.49
1:E:5004:SER:HB3	1:E:5012:THR:HG22	1.94	0.49
1:E:5031:VAL:HG13	1:E:5064:VAL:CG1	2.42	0.49
1:C:2029:GLU:O	1:C:2033:LYS:HE3	2.13	0.49
1:E:5049:GLU:HG3	1:E:5068:GLY:HA3	1.94	0.49
1:C:2147:ILE:HD13	1:C:2243:LYS:HE3	1.95	0.48
1:F:4012:THR:O	1:F:4015:ASP:HB2	2.12	0.48
1:D:3236:GLN:HE21	1:D:3236:GLN:CA	2.11	0.48
1:F:4234:MET:HB3	1:F:4238:GLU:HB2	1.95	0.48
1:F:4060:LYS:HB2	1:F:4253:LEU:HD13	1.95	0.48
1:C:2230:ASN:N	1:C:2230:ASN:HD22	2.10	0.48
1:F:4037:LEU:HD12	1:F:4246:VAL:HG21	1.96	0.48
1:C:2158:SER:CB	1:C:2200:ALA:HB2	2.37	0.48
1:D:3057:LEU:HD22	1:D:3250:ARG:HG3	1.96	0.48
1:F:4127:GLU:N	1:F:4127:GLU:OE1	2.47	0.48
1:D:3108:LEU:CD2	1:D:3152:HIS:HB2	2.43	0.48
1:E:5091:ARG:HG2	1:E:5215:MET:SD	2.54	0.48
1:A:1232:GLU:HA	1:A:1235:LYS:CB	2.41	0.48
1:C:2021:LEU:HD23	1:C:2022:ALA:N	2.29	0.48
1:E:5105:GLY:HA2	1:E:5237:THR:HG23	1.96	0.48
1:A:1024:VAL:O	1:A:1024:VAL:HG23	2.13	0.48
1:E:5114:VAL:HG12	1:E:5116:LEU:CD1	2.43	0.47
1:E:5119:ALA:HB3	1:E:5201:THR:OG1	2.14	0.47
1:A:1167:GLU:HG2	1:A:1169:TYR:CE1	2.48	0.47
1:A:1057:LEU:HD11	1:A:1250:ARG:HG2	1.95	0.47
1:C:2230:ASN:N	1:C:2230:ASN:ND2	2.60	0.47
1:E:5091:ARG:HD3	1:E:5215:MET:SD	2.54	0.47
1:A:1222:ASN:CB	1:A:1225:GLN:HE21	2.27	0.47
1:D:3028:PRO:HB3	1:D:3051:THR:HG23	1.96	0.47
1:B:6108:LEU:CD2	1:B:6152:HIS:HB2	2.44	0.47
1:C:2184:MET:O	1:C:2188:GLN:HG3	2.15	0.47
1:A:1108:LEU:CD2	1:A:1152:HIS:HB2	2.45	0.47
1:C:2027:ASP:OD1	1:C:2029:GLU:N	2.45	0.47
1:F:4234:MET:O	1:F:4238:GLU:HB3	2.14	0.47
1:E:5009:LEU:CD1	1:E:5081:LEU:HD13	2.45	0.47
1:E:5021:LEU:HD23	1:E:5021:LEU:C	2.35	0.47
1:E:5215:MET:HE2	4:E:9001:HOH:O	2.13	0.47
1:F:4156:THR:HG22	1:F:4194:ASN:OD1	2.14	0.47
1:C:2092:ILE:O	1:C:2092:ILE:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3024:VAL:O	1:D:3024:VAL:HG23	2.15	0.47
1:C:2102:ILE:O	1:C:2222:ASN:ND2	2.48	0.47
1:A:1093:GLY:O	1:A:1217:ALA:HA	2.14	0.47
1:B:6028:PRO:HA	1:B:6066:SER:HB3	1.97	0.47
1:E:5230:ASN:O	1:E:5233:THR:N	2.27	0.47
1:D:3137:THR:O	1:D:3141:VAL:HG23	2.15	0.47
1:E:5247:GLU:OE2	1:E:5247:GLU:HA	2.15	0.47
1:E:5016:LEU:HG	1:E:5063:ILE:HG13	1.97	0.47
1:B:6241:ALA:O	1:B:6244:ILE:HG12	2.15	0.46
1:E:5185:GLU:O	1:E:5185:GLU:HG2	2.15	0.46
1:C:2163:TYR:HB2	1:C:2164:PRO:CD	2.45	0.46
1:F:4092:ILE:O	1:F:4092:ILE:HG23	2.15	0.46
1:F:4221:VAL:HB	1:F:4229:PRO:HG3	1.97	0.46
1:F:4163:TYR:HB2	1:F:4164:PRO:CD	2.46	0.46
1:B:6199:SER:HB2	1:B:6203:LEU:HD22	1.98	0.46
1:C:2007:PHE:C	1:C:2007:PHE:CD2	2.88	0.46
1:D:3009:LEU:HD13	1:D:3080:GLU:OE1	2.16	0.46
1:A:1082:ALA:O	1:A:1087:ARG:NH2	2.49	0.46
1:A:1089:PHE:HE1	1:A:1211:LEU:HG	1.80	0.46
1:B:6145:LYS:O	1:B:6145:LYS:HD2	2.16	0.46
1:E:5082:ALA:O	1:E:5087:ARG:NH2	2.48	0.46
1:C:2105:GLY:HA2	1:C:2237:THR:HG22	1.97	0.46
1:D:3229:PRO:CB	1:D:3233:THR:HG21	2.46	0.46
1:F:4089:PHE:O	1:F:4213:ALA:HA	2.16	0.46
1:B:6163:TYR:HB2	1:B:6164:PRO:CD	2.46	0.46
1:F:4021:LEU:HD23	1:F:4022:ALA:N	2.30	0.46
1:E:5044:LEU:HD11	1:E:5054:ARG:NH1	2.31	0.46
1:E:5151:THR:HG22	1:E:5152:HIS:N	2.31	0.46
1:D:3205:MET:HB2	1:D:3205:MET:HE2	1.79	0.46
1:B:6238:GLU:H	1:B:6238:GLU:CD	2.19	0.46
1:A:1235:LYS:CG	1:A:1236:GLN:H	2.29	0.45
1:E:5092:ILE:HD13	1:E:5092:ILE:C	2.36	0.45
1:D:3104:VAL:HA	1:D:3219:VAL:CG1	2.47	0.45
1:F:4196:GLU:OE1	1:F:4199:SER:N	2.41	0.45
1:C:2169:TYR:O	1:C:2171:THR:N	2.50	0.45
1:C:2233:THR:H	1:C:2235:LYS:HD3	1.82	0.45
1:E:5232:GLU:O	1:E:5235:LYS:HB3	2.15	0.45
1:C:2234:MET:O	1:C:2238:GLU:HB3	2.16	0.45
1:D:3229:PRO:C	1:D:3233:THR:HG21	2.36	0.45
1:D:3237:THR:O	1:D:3240:HIS:HB3	2.16	0.45
1:C:2137:THR:O	1:C:2141:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3090:LEU:HD11	1:D:3252:LEU:HD12	1.98	0.45
1:E:5030:ARG:HB2	4:E:9120:HOH:O	2.17	0.45
1:F:4205:MET:O	1:F:4209:GLN:HB2	2.16	0.45
1:A:1107:VAL:HG21	1:A:1244:ILE:CD1	2.47	0.45
1:F:4038:MET:SD	1:F:4062:VAL:HG21	2.56	0.45
1:E:5030:ARG:O	1:E:5034:ILE:HG13	2.17	0.44
1:D:3021:LEU:HD23	1:D:3022:ALA:N	2.31	0.44
1:F:4028:PRO:HA	1:F:4066:SER:HB3	1.99	0.44
1:C:2077:ALA:O	1:C:2081:LEU:HB2	2.17	0.44
1:C:2086:ILE:O	1:C:2087:ARG:NH1	2.50	0.44
1:E:5081:LEU:HA	1:E:5081:LEU:HD12	1.74	0.44
1:C:2024:VAL:HG23	1:C:2024:VAL:O	2.17	0.44
1:B:6201:THR:O	1:B:6205:MET:HG2	2.17	0.44
1:F:4242:VAL:O	1:F:4245:VAL:HG12	2.18	0.44
1:F:4048:ARG:HB3	1:F:4049:GLU:OE2	2.18	0.44
1:C:2092:ILE:C	1:C:2092:ILE:HD13	2.37	0.44
1:C:2157:ALA:HB2	1:C:2192:VAL:HG11	1.98	0.44
1:F:4038:MET:HB2	1:F:4055:ALA:HB1	2.00	0.44
1:B:6095:THR:OG1	1:B:6194:ASN:HB2	2.18	0.44
1:F:4235:LYS:HZ2	1:F:4235:LYS:HB2	1.81	0.44
1:A:1016:LEU:HG	1:A:1063:ILE:HG13	1.99	0.44
1:C:2040:LYS:HD2	1:C:2040:LYS:H	1.78	0.44
1:D:3201:THR:O	1:D:3205:MET:HG2	2.17	0.44
1:F:4103:ASN:O	1:F:4106:ASP:HB2	2.17	0.44
1:E:5024:VAL:O	1:E:5024:VAL:HG23	2.18	0.44
1:D:3091:ARG:HG3	1:D:3091:ARG:HH11	1.82	0.44
1:D:3236:GLN:NE2	1:D:3236:GLN:CA	2.78	0.43
1:F:4005:ASP:HB2	1:F:4012:THR:HA	1.99	0.43
1:F:4049:GLU:N	1:F:4049:GLU:OE2	2.44	0.43
1:E:5230:ASN:HB2	1:E:5233:THR:HG1	1.82	0.43
1:C:2238:GLU:O	1:C:2242:VAL:HG23	2.17	0.43
1:D:3175:ARG:NH2	1:F:4190:MET:HG2	2.33	0.43
1:F:4056:GLU:HA	1:F:4060:LYS:O	2.19	0.43
1:D:3089:PHE:O	1:D:3213:ALA:HA	2.19	0.43
1:F:4031:VAL:HG13	1:F:4064:VAL:CG1	2.48	0.43
1:C:2030:ARG:NE	1:C:2238:GLU:OE2	2.49	0.43
1:E:5241:ALA:O	1:E:5244:ILE:HB	2.18	0.43
1:A:1169:TYR:CE2	1:A:1176:VAL:HG23	2.54	0.43
1:E:5247:GLU:OE1	1:E:5251:ARG:NH1	2.47	0.43
1:C:2057:LEU:HB3	1:C:2253:LEU:HD11	2.01	0.43
1:B:6196:GLU:CD	1:B:6199:SER:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2038:MET:HB3	1:C:2056:GLU:O	2.19	0.43
1:F:4102:ILE:O	1:F:4222:ASN:ND2	2.50	0.43
1:E:5067:THR:HB	1:E:5074:THR:HA	2.00	0.43
1:F:4158:SER:HA	1:F:4196:GLU:O	2.19	0.43
1:C:2033:LYS:O	1:C:2036:ALA:HB3	2.18	0.43
1:C:2158:SER:HB3	1:C:2200:ALA:CB	2.38	0.43
1:C:2007:PHE:O	1:C:2007:PHE:HD2	2.01	0.43
1:D:3016:LEU:HG	1:D:3063:ILE:HG13	2.00	0.43
1:C:2160:ASP:O	1:E:5072:PRO:HA	2.18	0.43
1:E:5110:THR:OG1	1:E:5156:THR:HG21	2.19	0.42
1:D:3030:ARG:NH1	1:D:3092:ILE:O	2.52	0.42
1:D:3199:SER:O	1:D:3203:LEU:HG	2.18	0.42
1:F:4086:ILE:O	1:F:4087:ARG:HD2	2.19	0.42
1:A:1049:GLU:HG3	1:A:1068:GLY:HA3	2.00	0.42
1:E:5057:LEU:HB3	1:E:5253:LEU:CD2	2.49	0.42
1:D:3048:ARG:HB3	1:D:3049:GLU:OE2	2.20	0.42
1:A:1220:ILE:CB	1:A:1233:THR:HG23	2.42	0.42
1:E:5022:ALA:HA	1:E:5063:ILE:O	2.20	0.42
1:F:4025:PRO:O	1:F:4066:SER:HA	2.19	0.42
1:A:1060:LYS:CG	1:A:1253:LEU:HD13	2.49	0.42
1:C:2211:LEU:HD21	1:E:5172:TYR:CE1	2.55	0.42
1:A:1235:LYS:HG3	1:A:1236:GLN:N	2.34	0.42
1:B:6035:ALA:HA	1:B:6038:MET:HE3	2.02	0.42
1:C:2012:THR:H	1:C:2015:ASP:HB2	1.84	0.42
1:E:5158:SER:CB	1:E:5200:ALA:HB2	2.43	0.41
1:C:2027:ASP:HA	1:C:2028:PRO:HD3	1.89	0.41
1:C:2234:MET:O	1:C:2238:GLU:CB	2.68	0.41
1:B:6248:ALA:HA	1:B:6251:ARG:HD2	2.02	0.41
1:A:1071:GLY:N	1:A:1072:PRO:CD	2.83	0.41
1:C:2247:GLU:O	1:C:2250:ARG:HB2	2.20	0.41
1:C:2017:GLN:HB2	1:C:2054:ARG:HD2	2.02	0.41
1:D:3125:PRO:HB2	1:D:3127:GLU:OE2	2.20	0.41
1:D:3077:ALA:O	1:D:3081:LEU:HB2	2.20	0.41
1:C:2071:GLY:N	1:C:2072:PRO:CD	2.84	0.41
1:A:1232:GLU:CA	1:A:1232:GLU:OE2	2.69	0.41
1:D:3049:GLU:HG3	1:D:3068:GLY:HA3	2.01	0.41
1:D:3081:LEU:HA	1:D:3081:LEU:HD12	1.94	0.41
1:A:1203:LEU:HA	1:A:1203:LEU:HD12	1.84	0.41
1:D:3194:ASN:OD1	1:D:3194:ASN:N	2.53	0.41
1:B:6243:LYS:HD3	1:B:6243:LYS:O	2.21	0.41
1:C:2031:VAL:HG21	1:C:2051:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:ILE:O	1:A:1092:ILE:HG23	2.21	0.41
1:F:4163:TYR:HB2	1:F:4164:PRO:HD3	2.02	0.41
1:A:1070:GLY:HA3	1:F:4072:PRO:HB2	2.02	0.41
1:C:2172:TYR:CE1	1:E:5211:LEU:HD11	2.55	0.41
1:E:5057:LEU:HD12	1:E:5057:LEU:HA	1.86	0.41
1:D:3046:SER:OG	1:D:3051:THR:HG22	2.21	0.41
1:C:2024:VAL:HA	1:C:2025:PRO:HD2	1.97	0.41
1:E:5199:SER:HB3	1:E:5215:MET:SD	2.60	0.40
1:A:1233:THR:C	1:A:1235:LYS:H	2.24	0.40
1:C:2216:VAL:HG22	1:C:2217:ALA:N	2.36	0.40
1:E:5196:GLU:HG2	1:E:5215:MET:HE1	2.03	0.40
1:A:1012:THR:O	1:A:1015:ASP:HB2	2.20	0.40
1:A:1010:GLY:HA3	1:A:1047:HIS:CD2	2.56	0.40
1:C:2126:MET:HG3	1:D:3126:MET:HG3	2.04	0.40
1:F:4024:VAL:HB	1:F:4067:THR:CG2	2.51	0.40
1:E:5107:VAL:O	1:E:5151:THR:HA	2.22	0.40
1:B:6249:ALA:O	1:B:6253:LEU:HG	2.22	0.40
1:B:6234:MET:SD	1:B:6234:MET:C	3.00	0.40
1:D:3017:GLN:HA	1:D:3017:GLN:HE21	1.86	0.40
1:D:3006:VAL:HG21	1:D:3009:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/253 (98%)	232 (94%)	12 (5%)	4 (2%)	12	20
1	B	248/253 (98%)	221 (89%)	23 (9%)	4 (2%)	12	20
1	C	248/253 (98%)	225 (91%)	20 (8%)	3 (1%)	16	27
1	D	248/253 (98%)	230 (93%)	12 (5%)	6 (2%)	7	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	248/253 (98%)	230 (93%)	15 (6%)	3 (1%)	16	27
1	F	248/253 (98%)	230 (93%)	17 (7%)	1 (0%)	39	60
All	All	1488/1518 (98%)	1368 (92%)	99 (7%)	21 (1%)	14	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2230	ASN
1	C	2235	LYS
1	D	3005	ASP
1	E	5231	ALA
1	B	6233	THR
1	A	1163	TYR
1	A	1233	THR
1	D	3229	PRO
1	D	3231	ALA
1	B	6163	TYR
1	B	6232	GLU
1	B	6236	GLN
1	A	1230	ASN
1	D	3163	TYR
1	E	5163	TYR
1	E	5229	PRO
1	C	2163	TYR
1	D	3148	GLY
1	D	3233	THR
1	F	4163	TYR
1	A	1232	GLU

### 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	199/202 (98%)	187 (94%)	12 (6%)	24	41
1	B	199/202 (98%)	187 (94%)	12 (6%)	24	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	199/202 (98%)	187 (94%)	12 (6%)	24	41
1	D	199/202 (98%)	185 (93%)	14 (7%)	19	33
1	E	199/202 (98%)	183 (92%)	16 (8%)	15	26
1	F	199/202 (98%)	186 (94%)	13 (6%)	21	37
All	All	1194/1212 (98%)	1115 (93%)	79 (7%)	21	36

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1091	ARG
1	A	1092	ILE
1	A	1127	GLU
1	A	1146	SER
1	A	1160	ASP
1	A	1179	ARG
1	A	1193	MET
1	A	1198	GLU
1	A	1203	LEU
1	A	1211	LEU
1	A	1227	GLU
1	A	1234	MET
1	C	2009	LEU
1	C	2049	GLU
1	C	2052	SER
1	C	2091	ARG
1	C	2092	ILE
1	C	2102	ILE
1	C	2185	GLU
1	C	2196	GLU
1	C	2228	ILE
1	C	2230	ASN
1	C	2232	GLU
1	C	2251	ARG
1	D	3014	ASN
1	D	3017	GLN
1	D	3037	LEU
1	D	3081	LEU
1	D	3092	ILE
1	D	3103	ASN
1	D	3133	ASP
1	D	3147	ILE

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Mol	Chain	Res	Type
1	D	3160	ASP
1	D	3178	ARG
1	D	3184	MET
1	D	3229	PRO
1	D	3230	ASN
1	D	3236	GLN
1	F	4033	LYS
1	F	4087	ARG
1	F	4127	GLU
1	F	4175	ARG
1	F	4179	ARG
1	F	4193	MET
1	F	4215	MET
1	F	4228	ILE
1	F	4229	PRO
1	F	4230	ASN
1	F	4233	THR
1	F	4234	MET
1	F	4239	SER
1	E	5014	ASN
1	E	5017	GLN
1	E	5044	LEU
1	E	5081	LEU
1	E	5091	ARG
1	E	5092	ILE
1	E	5116	LEU
1	E	5142	GLU
1	E	5156	THR
1	E	5170	ASP
1	E	5177	VAL
1	E	5179	ARG
1	E	5203	LEU
1	E	5211	LEU
1	E	5224	THR
1	E	5233	THR
1	B	6011	LEU
1	B	6092	ILE
1	B	6145	LYS
1	B	6153	VAL
1	B	6170	ASP
1	B	6184	MET
1	B	6201	THR

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Mol	Chain	Res	Type
1	B	6203	LEU
1	B	6230	ASN
1	B	6233	THR
1	B	6234	MET
1	B	6236	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1014	ASN
1	A	1225	GLN
1	C	2152	HIS
1	C	2230	ASN
1	D	3017	GLN
1	D	3103	ASN
1	D	3236	GLN
1	F	4226	GLN
1	F	4236	GLN
1	E	5014	ASN
1	B	6103	ASN
1	B	6225	GLN
1	B	6226	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 ⓘ

11 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	SO4	A	7001	-	4,4,4	0.29	0	6,6,6	0.17	0
3	URA	A	8001	-	4,8,8	3.44	2 (50%)	6,10,10	11.57	4 (66%)
2	SO4	B	7006	-	4,4,4	0.25	0	6,6,6	0.13	0
3	URA	B	8006	-	4,8,8	3.19	2 (50%)	6,10,10	11.49	4 (66%)
2	SO4	C	7002	-	4,4,4	0.32	0	6,6,6	0.13	0
2	SO4	D	7003	-	4,4,4	0.20	0	6,6,6	0.10	0
3	URA	D	8003	-	4,8,8	3.37	2 (50%)	6,10,10	11.44	4 (66%)
2	SO4	E	7005	-	4,4,4	0.20	0	6,6,6	0.09	0
3	URA	E	8005	-	4,8,8	3.55	2 (50%)	6,10,10	11.45	4 (66%)
2	SO4	F	7004	-	4,4,4	0.23	0	6,6,6	0.06	0
3	URA	F	8004	-	4,8,8	3.53	2 (50%)	6,10,10	11.55	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	SO4	A	7001	-	-	0/0/0/0	0/0/0/0
3	URA	A	8001	-	-	0/0/0/0	0/1/1/1
2	SO4	B	7006	-	-	0/0/0/0	0/0/0/0
3	URA	B	8006	-	-	0/0/0/0	0/1/1/1
2	SO4	C	7002	-	-	0/0/0/0	0/0/0/0
2	SO4	D	7003	-	-	0/0/0/0	0/0/0/0
3	URA	D	8003	-	-	0/0/0/0	0/1/1/1
2	SO4	E	7005	-	-	0/0/0/0	0/0/0/0
3	URA	E	8005	-	-	0/0/0/0	0/1/1/1
2	SO4	F	7004	-	-	0/0/0/0	0/0/0/0
3	URA	F	8004	-	-	0/0/0/0	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	8003	URA	C6-N1	3.57	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	8006	URA	C6-N1	3.65	1.42	1.34
3	F	8004	URA	C6-N1	3.67	1.42	1.34
3	A	8001	URA	C6-N1	3.70	1.42	1.34
3	E	8005	URA	C6-N1	3.73	1.42	1.34
3	B	8006	URA	C4-N3	4.88	1.42	1.33
3	D	8003	URA	C4-N3	5.36	1.43	1.33
3	A	8001	URA	C4-N3	5.54	1.43	1.33
3	E	8005	URA	C4-N3	5.73	1.43	1.33
3	F	8004	URA	C4-N3	5.81	1.43	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	8001	URA	N1-C2-N3	-21.22	114.80	128.33
3	B	8006	URA	N1-C2-N3	-21.06	114.90	128.33
3	F	8004	URA	N1-C2-N3	-21.02	114.92	128.33
3	D	8003	URA	N1-C2-N3	-20.83	115.04	128.33
3	E	8005	URA	N1-C2-N3	-20.81	115.05	128.33
3	F	8004	URA	C5-C4-N3	-3.36	114.50	123.12
3	D	8003	URA	C5-C4-N3	-3.36	114.51	123.12
3	A	8001	URA	C5-C4-N3	-3.30	114.64	123.12
3	B	8006	URA	C5-C4-N3	-3.27	114.73	123.12
3	E	8005	URA	C5-C4-N3	-3.21	114.88	123.12
3	E	8005	URA	C4-N3-C2	12.32	126.34	114.14
3	D	8003	URA	C4-N3-C2	12.60	126.62	114.14
3	F	8004	URA	C4-N3-C2	12.73	126.75	114.14
3	A	8001	URA	C4-N3-C2	12.75	126.77	114.14
3	B	8006	URA	C6-N1-C2	12.92	120.75	114.40
3	B	8006	URA	C4-N3-C2	12.97	126.99	114.14
3	A	8001	URA	C6-N1-C2	13.29	120.94	114.40
3	D	8003	URA	C6-N1-C2	13.34	120.96	114.40
3	F	8004	URA	C6-N1-C2	13.48	121.03	114.40
3	E	8005	URA	C6-N1-C2	13.72	121.15	114.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/253 (98%)	-0.34	5 (2%) 68 73	6, 19, 45, 92	0
1	B	250/253 (98%)	-0.24	8 (3%) 51 57	6, 20, 43, 109	0
1	C	250/253 (98%)	0.01	15 (6%) 25 29	6, 25, 58, 104	0
1	D	250/253 (98%)	-0.16	9 (3%) 46 53	7, 22, 52, 133	0
1	E	250/253 (98%)	-0.18	10 (4%) 42 48	7, 21, 51, 100	0
1	F	250/253 (98%)	-0.23	7 (2%) 56 62	5, 20, 45, 120	0
All	All	1500/1518 (98%)	-0.19	54 (3%) 46 53	5, 21, 52, 133	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1234	MET	12.6
1	D	3231	ALA	8.8
1	D	3230	ASN	8.7
1	B	6234	MET	8.0
1	C	2230	ASN	7.4
1	F	4230	ASN	6.8
1	E	5228	ILE	6.5
1	D	3228	ILE	6.1
1	E	5227	GLU	5.9
1	C	2231	ALA	5.9
1	F	4229	PRO	5.8
1	F	4233	THR	5.7
1	B	6236	GLN	5.7
1	F	4232	GLU	5.4
1	E	5226	GLN	5.2
1	B	6231	ALA	5.1
1	F	4231	ALA	5.0
1	D	3229	PRO	4.6
1	E	5231	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	6237	THR	4.5
1	B	6233	THR	4.4
1	E	5229	PRO	4.0
1	D	3232	GLU	4.0
1	C	2229	PRO	4.0
1	C	2234	MET	4.0
1	F	4228	ILE	3.9
1	C	2226	GLN	3.6
1	C	2221	VAL	3.5
1	D	3226	GLN	3.5
1	D	3233	THR	3.2
1	A	1231	ALA	3.2
1	B	6238	GLU	3.0
1	C	2233	THR	2.9
1	C	2101	HIS	2.9
1	C	2235	LYS	2.9
1	F	4234	MET	2.9
1	E	5230	ASN	2.8
1	B	6235	LYS	2.8
1	D	3004	SER	2.6
1	A	1236	GLN	2.6
1	C	2227	GLU	2.4
1	C	2148	GLY	2.4
1	E	5234	MET	2.4
1	E	5145	LYS	2.3
1	A	1227	GLU	2.3
1	B	6232	GLU	2.3
1	C	2007	PHE	2.2
1	E	5232	GLU	2.2
1	A	1235	LYS	2.1
1	C	2225	GLN	2.1
1	D	3235	LYS	2.1
1	E	5233	THR	2.1
1	C	2104	VAL	2.0
1	C	2090	LEU	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	7002	5/5	0.94	0.19	0.58	48,60,62,68	0
3	URA	E	8005	8/8	0.94	0.17	0.55	29,34,39,43	0
2	SO4	B	7006	5/5	0.99	0.15	0.50	12,14,31,46	0
3	URA	B	8006	8/8	0.97	0.12	0.12	7,14,19,33	0
3	URA	F	8004	8/8	0.96	0.12	-0.15	4,6,17,19	0
2	SO4	F	7004	5/5	0.99	0.14	-0.23	16,24,27,50	0
3	URA	D	8003	8/8	0.97	0.12	-0.68	18,26,31,31	0
3	URA	A	8001	8/8	0.98	0.09	-0.95	10,15,19,24	0
2	SO4	E	7005	5/5	0.99	0.12	-0.96	28,29,39,50	0
2	SO4	D	7003	5/5	0.99	0.11	-1.70	18,26,31,40	0
2	SO4	A	7001	5/5	0.99	0.07	-1.82	6,7,23,48	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.