



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:21 AM GMT

PDB ID : 2QDK  
Title : X-ray structure of the unliganded uridine phosphorylase from *Salmonella typhimurium* at 1.62Å resolution  
Authors : Timofeev, V.I.; Pavlyuk, B.P.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Mikhailov, A.M.  
Deposited on : 2007-06-21  
Resolution : 1.62 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

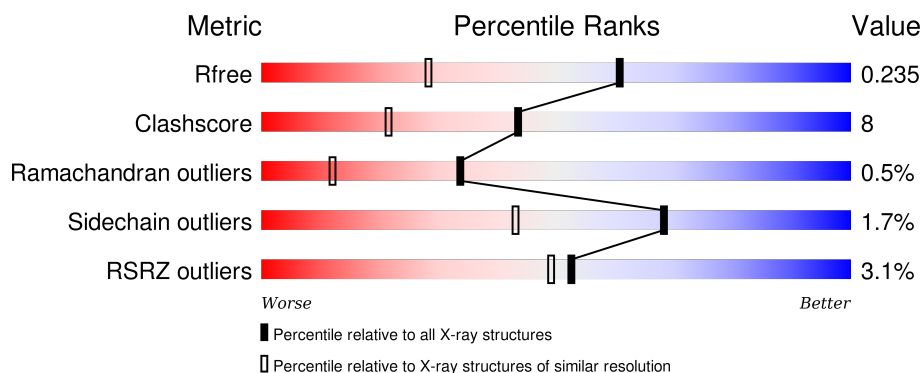
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.62 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	3202 (1.64-1.60)
Clashscore	102246	3500 (1.64-1.60)
Ramachandran outliers	100387	3411 (1.64-1.60)
Sidechain outliers	100360	3410 (1.64-1.60)
RSRZ outliers	91569	3207 (1.64-1.60)

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	252	<div> <div>4%</div> <div>85%15%</div> </div>
1	B	252	<div> <div>%</div> <div>77%17%6%</div> </div>
1	C	252	<div> <div>4%</div> <div>81%13%5%</div> </div>
1	D	252	<div> <div>2%</div> <div>88%8%..</div> </div>
1	E	252	<div> <div>5%</div> <div>82%15%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	252	<div><div></div><div>2%</div><div>83%</div><div>14%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12851 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	252	Total	C	N	O	S	0	18	0
			1994	1256	343	381	14			
1	B	238	Total	C	N	O	S	0	15	0
			1876	1186	331	347	12			
1	C	240	Total	C	N	O	S	0	11	0
			1866	1173	328	354	11			
1	D	244	Total	C	N	O	S	0	11	0
			1899	1196	332	360	11			
1	E	248	Total	C	N	O	S	0	12	0
			1934	1217	341	364	12			
1	F	245	Total	C	N	O	S	0	12	0
			1901	1201	330	358	12			

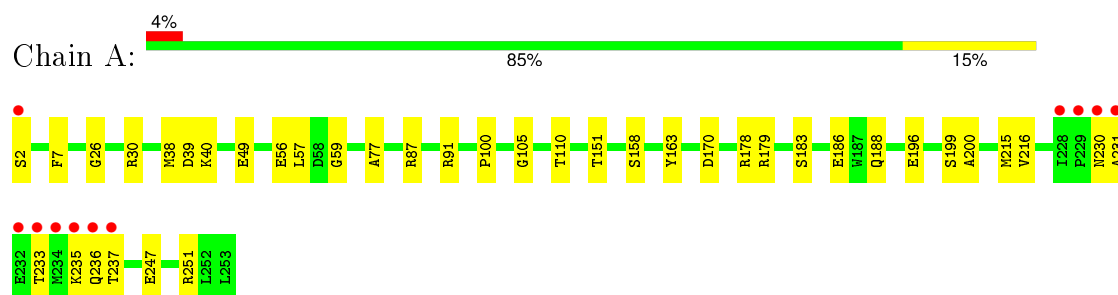
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	246	Total	O	0	5
			250	250		
2	B	215	Total	O	0	0
			215	215		
2	C	221	Total	O	0	2
			223	223		
2	D	210	Total	O	0	3
			212	212		
2	E	252	Total	O	0	1
			253	253		
2	F	224	Total	O	0	3
			228	228		

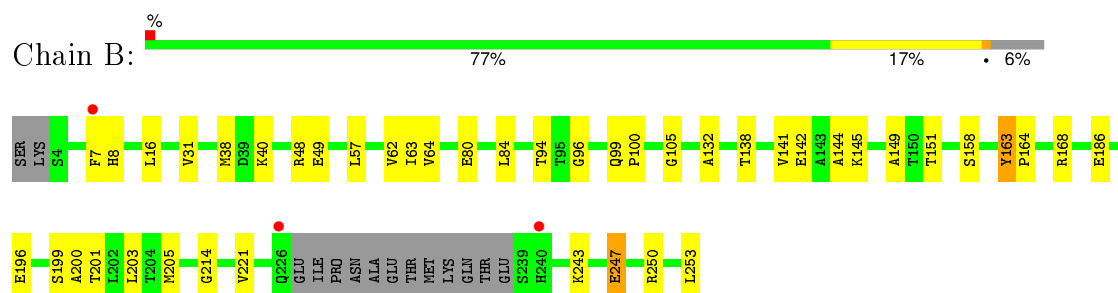
### 3 Residue-property plots [i](#)

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

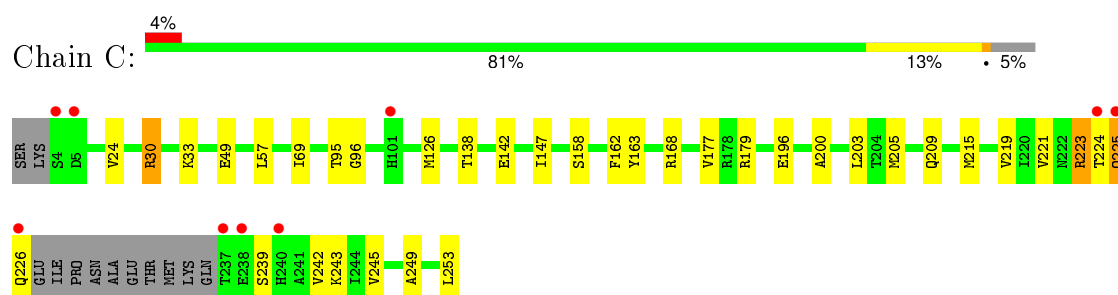
- Molecule 1: Uridine phosphorylase



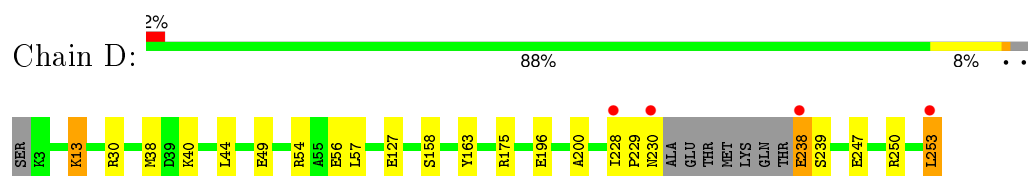
- Molecule 1: Uridine phosphorylase



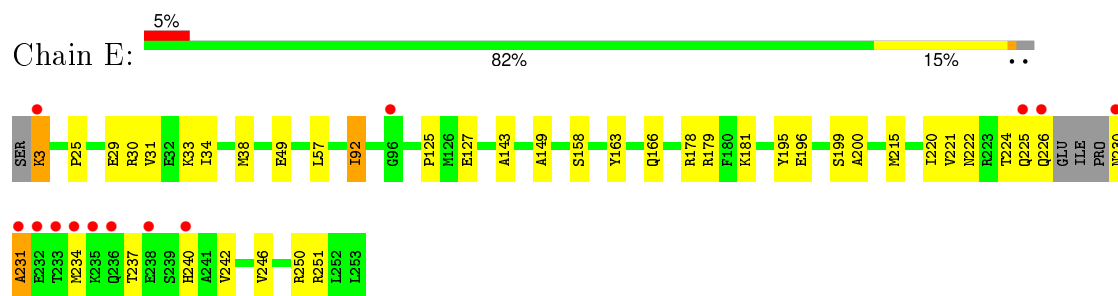
- Molecule 1: Uridine phosphorylase



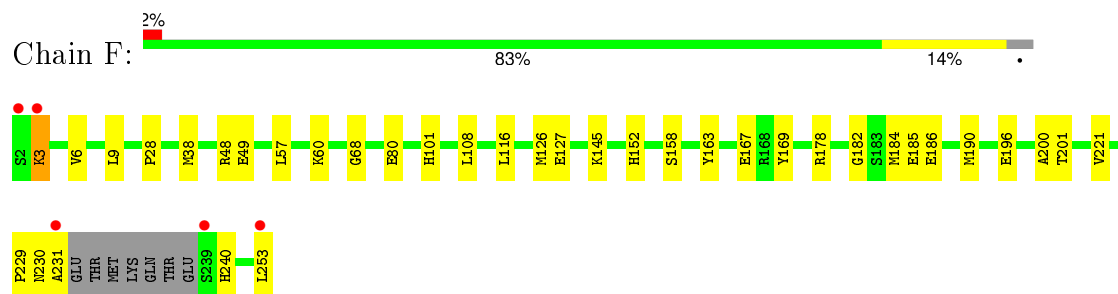
- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



- Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.60Å 125.03Å 134.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.62 6.00 – 1.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.62) 95.7 (6.00-1.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 1.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.191 , (Not available) 0.184 , 0.235	Depositor DCC
$R_{free}$ test set	9000 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	1.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.66 , 80.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 180015 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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

### 5.1 Standard geometry

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	0.39	0/2079	0.57	0/2812
1	B	0.34	0/1950	0.54	0/2632
1	C	0.35	0/1927	0.55	0/2606
1	D	0.36	0/1963	0.57	0/2656
1	E	0.39	0/2000	0.57	0/2703
1	F	0.38	0/1967	0.56	0/2660
All	All	0.37	0/11886	0.56	0/16069

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

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	1994	0	2050	32	0
1	B	1876	0	1944	38	0
1	C	1866	0	1906	37	0
1	D	1899	0	1930	20	0
1	E	1934	0	1980	41	0
1	F	1901	0	1952	28	0
2	A	250	0	0	11	0
2	B	215	0	0	11	0
2	C	223	0	0	14	0
2	D	212	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	253	0	0	10	0
2	F	228	0	0	8	0
All	All	12851	0	11762	188	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 (188) 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:A:39[B]:ASP:HB3	1:A:56[B]:GLU:HG3	1.25	1.08
1:C:179:ARG:HB3	2:C:448:HOH:O	1.57	1.01
1:E:25:PRO:HG3	2:E:486:HOH:O	1.65	0.96
1:A:39[B]:ASP:HB3	1:A:56[B]:GLU:CG	2.00	0.90
1:D:229:PRO:HA	1:D:230:ASN:C	1.90	0.90
1:E:34:ILE:HD12	2:E:486:HOH:O	1.74	0.88
1:E:149:ALA:HB2	1:E:240[B]:HIS:HE1	1.39	0.86
1:E:149:ALA:HB2	1:E:240[B]:HIS:CE1	2.10	0.85
1:C:225:GLN:O	1:C:226:GLN:HB2	1.78	0.83
1:E:149:ALA:CB	1:E:240[B]:HIS:HE1	1.94	0.81
1:A:91:ARG:HD3	2:A:460:HOH:O	1.81	0.79
1:F:201:THR:HB	2:F:455:HOH:O	1.81	0.79
1:C:223:ARG:HH11	1:C:223:ARG:CG	1.98	0.77
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.51	0.76
1:C:177:VAL:HG13	2:C:448:HOH:O	1.85	0.75
1:C:225:GLN:O	1:C:226:GLN:CB	2.34	0.74
1:B:144:ALA:HB1	1:B:151:THR:HG21	1.70	0.74
1:C:224:THR:O	1:C:225:GLN:HG3	1.87	0.73
1:E:178:ARG:HA	1:E:181:LYS:HE2	1.71	0.73
1:E:230:ASN:HA	2:E:483:HOH:O	1.88	0.72
1:E:30[A]:ARG:NH1	1:E:33:LYS:HD3	2.04	0.72
1:E:225:GLN:O	1:E:226:GLN:HB2	1.91	0.70
1:C:223:ARG:NH1	1:C:223:ARG:HG2	2.05	0.68
1:B:141:VAL:O	1:B:145[B]:LYS:HG2	1.94	0.67
1:E:179:ARG:NH2	2:E:475:HOH:O	2.28	0.66
2:C:434:HOH:O	1:F:49:GLU:HB2	1.94	0.66
1:A:56[B]:GLU:OE1	1:A:59:GLY:HA2	1.96	0.66
1:F:184[B]:MET:HE2	2:F:440:HOH:O	1.94	0.65
1:E:3:LYS:HE2	1:E:3:LYS:N	2.10	0.65
1:B:57:LEU:HD21	1:B:250[B]:ARG:HG2	1.77	0.65
1:F:221:VAL:HB	1:F:229:PRO:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30[A]:ARG:CZ	1:E:33:LYS:HD3	2.27	0.64
1:C:95:THR:O	1:C:219:VAL:HA	1.98	0.64
1:C:215:MET:HB3	2:C:444:HOH:O	1.97	0.64
1:C:147:ILE:HG21	1:C:243[A]:LYS:HD3	1.80	0.63
1:C:224:THR:C	1:C:225:GLN:HG3	2.15	0.63
1:B:214:GLY:HA2	2:B:456:HOH:O	1.98	0.62
1:A:38:MET:HG2	1:A:57:LEU:HD13	1.80	0.62
1:E:30[B]:ARG:HH12	1:E:92[B]:ILE:HG13	1.65	0.62
1:B:84:LEU:HD13	2:B:438:HOH:O	1.99	0.61
1:D:238:GLU:CD	1:D:238:GLU:N	2.53	0.61
1:F:6:VAL:HG21	2:F:469:HOH:O	2.01	0.60
1:E:30[A]:ARG:NH2	1:E:242:VAL:HG21	2.16	0.60
1:A:178:ARG:HB2	1:F:186[A]:GLU:OE2	2.01	0.60
1:A:39[B]:ASP:OD1	1:A:40:LYS:HG2	2.02	0.59
1:A:199:SER:HA	2:A:460:HOH:O	2.02	0.59
1:E:30[B]:ARG:HH12	1:E:92[B]:ILE:CG1	2.16	0.58
1:F:60:LYS:HB2	1:F:253:LEU:HD13	1.85	0.58
1:D:238:GLU:OE2	1:D:238:GLU:N	2.37	0.58
1:B:57:LEU:HB3	1:B:253:LEU:HD11	1.86	0.58
1:E:30[A]:ARG:HH21	1:E:242:VAL:HG21	1.70	0.57
1:C:177:VAL:CG1	2:C:448:HOH:O	2.49	0.57
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.86	0.57
1:A:231:ALA:O	1:A:235:LYS:HG2	2.04	0.56
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.87	0.56
1:D:229:PRO:CA	1:D:230:ASN:C	2.70	0.56
1:C:239:SER:O	1:C:243[B]:LYS:HG3	2.06	0.56
1:B:57:LEU:CD2	1:B:250[B]:ARG:HG2	2.36	0.56
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.88	0.55
1:E:246:VAL:O	1:E:250[B]:ARG:HG3	2.06	0.55
1:E:234:MET:HE2	2:E:483:HOH:O	2.06	0.55
1:D:30[B]:ARG:NH2	2:D:354:HOH:O	2.40	0.54
1:C:203:LEU:HD21	2:C:444:HOH:O	2.06	0.54
1:A:30:ARG:CZ	2:A:351:HOH:O	2.56	0.54
1:F:230:ASN:O	1:F:231:ALA:CB	2.55	0.54
1:F:127:GLU:CD	1:F:127:GLU:H	2.11	0.54
1:B:94:THR:HG22	2:B:374:HOH:O	2.07	0.54
1:B:168:ARG:HD2	2:B:282:HOH:O	2.08	0.53
1:B:16:LEU:HD13	2:B:438:HOH:O	2.07	0.53
1:B:38:MET:SD	1:B:62:VAL:HG21	2.49	0.53
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.90	0.53
1:D:40:LYS:HD3	1:D:56[B]:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:HB2	1:D:228:ILE:HD11	1.91	0.53
1:A:158:SER:HB3	1:A:200:ALA:HB2	1.90	0.52
1:A:77:ALA:HB1	2:A:487:HOH:O	2.08	0.52
1:D:127[A]:GLU:HB2	2:D:439:HOH:O	2.08	0.52
1:D:238:GLU:HA	2:D:445:HOH:O	2.08	0.52
1:C:223:ARG:HD2	2:C:318:HOH:O	2.09	0.52
1:C:203:LEU:HD11	2:C:444:HOH:O	2.10	0.52
1:A:236:GLN:HG2	2:A:484:HOH:O	2.10	0.52
1:C:162:PHE:HE1	1:C:168[B]:ARG:NH2	2.08	0.51
1:F:38:MET:HG2	1:F:57[A]:LEU:HD13	1.92	0.51
1:A:91:ARG:HB3	1:A:215[B]:MET:HG3	1.91	0.51
1:F:9:LEU:HD12	2:F:469:HOH:O	2.10	0.51
1:C:138:THR:O	1:C:142[B]:GLU:HG2	2.11	0.51
1:B:144:ALA:CB	1:B:151:THR:HG21	2.40	0.51
1:F:182:GLY:O	1:F:185[B]:GLU:HG3	2.09	0.51
2:C:434:HOH:O	1:F:68:GLY:HA2	2.10	0.51
1:E:222:ASN:OD1	1:E:224:THR:HG22	2.11	0.51
1:E:3:LYS:CE	1:E:3:LYS:N	2.74	0.51
2:D:439:HOH:O	1:F:116:LEU:HD21	2.10	0.51
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.93	0.51
1:A:247:GLU:HG3	1:A:251[A]:ARG:HH12	1.77	0.50
1:C:96:GLY:HA2	1:C:221:VAL:O	2.11	0.50
1:A:151[B]:THR:HG21	2:A:326:HOH:O	2.12	0.50
1:B:49[A]:GLU:CG	1:E:49:GLU:HB3	2.41	0.50
1:B:94:THR:HG23	2:B:442:HOH:O	2.11	0.49
1:B:186:GLU:CD	1:F:178:ARG:HH21	2.15	0.49
1:C:223:ARG:HH11	1:C:223:ARG:CB	2.25	0.49
1:E:31:VAL:HA	2:E:486:HOH:O	2.12	0.49
1:C:30[A]:ARG:HD3	2:C:364:HOH:O	2.13	0.49
1:A:110:THR:OG1	1:A:215[B]:MET:HE3	2.13	0.48
1:B:7[A]:PHE:HD2	1:B:8:HIS:CE1	2.32	0.48
1:E:251:ARG:NH2	2:E:488:HOH:O	2.41	0.48
1:C:162:PHE:CE1	1:C:168[B]:ARG:NH2	2.81	0.47
1:B:149:ALA:O	1:B:151:THR:HG23	2.15	0.47
1:F:108:LEU:HD22	1:F:152:HIS:HB2	1.96	0.47
1:C:223:ARG:HG3	2:C:345:HOH:O	2.13	0.47
1:B:31:VAL:HG13	1:B:64:VAL:HG12	1.96	0.47
1:A:100:PRO:HD3	1:A:188[B]:GLN:HE21	1.79	0.47
1:A:247:GLU:HG3	1:A:251[A]:ARG:NH1	2.30	0.47
1:E:29:GLU:HB3	2:E:496:HOH:O	2.14	0.47
1:D:247:GLU:OE2	1:D:250[A]:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLU:HB3	1:F:49:GLU:HB3	1.97	0.46
1:B:105:GLY:HA3	2:B:441:HOH:O	2.14	0.46
1:E:3:LYS:HZ3	1:E:3:LYS:N	2.13	0.46
1:C:249:ALA:O	1:C:253:LEU:HG	2.15	0.46
1:B:203:LEU:HD22	2:B:456:HOH:O	2.15	0.46
1:B:138:THR:O	1:B:142[B]:GLU:HG3	2.16	0.45
1:D:127[B]:GLU:HB2	2:D:439:HOH:O	2.17	0.45
1:B:201:THR:O	1:B:205:MET:HG2	2.17	0.45
1:E:220:ILE:HG21	1:E:234:MET:HG3	1.97	0.45
1:B:203:LEU:CD2	2:B:456:HOH:O	2.63	0.45
1:C:69:ILE:HD11	1:F:48:ARG:HD3	1.99	0.45
1:D:38:MET:HG2	1:D:57:LEU:HD13	1.98	0.45
1:C:205:MET:O	1:C:209[B]:GLN:HG2	2.17	0.45
1:D:13:LYS:HB2	1:D:13:LYS:HE2	1.58	0.44
1:C:126:MET:HE1	2:C:460:HOH:O	2.16	0.44
2:C:434:HOH:O	1:F:28:PRO:HD3	2.16	0.44
1:E:143:ALA:HA	2:E:488:HOH:O	2.17	0.44
1:A:49:GLU:HB3	1:D:49:GLU:HB3	1.99	0.44
1:C:168[B]:ARG:HG2	1:C:223:ARG:NH2	2.32	0.44
1:E:125:PRO:HB2	1:E:127[B]:GLU:OE1	2.17	0.44
1:B:243:LYS:HD2	2:B:447:HOH:O	2.16	0.44
1:F:80:GLU:HB3	2:F:469:HOH:O	2.17	0.44
1:C:57:LEU:HB3	1:C:253:LEU:HD11	1.99	0.44
1:A:247:GLU:OE2	1:A:251[B]:ARG:NH2	2.50	0.44
1:A:2:SER:HA	2:A:452:HOH:O	2.17	0.44
1:B:132:ALA:CB	2:B:456:HOH:O	2.65	0.44
1:A:230:ASN:OD1	1:A:233:THR:HG22	2.18	0.44
1:B:141:VAL:CG1	1:B:145[B]:LYS:HE2	2.48	0.43
1:E:222:ASN:HB3	1:E:225:GLN:HB2	2.00	0.43
1:E:38:MET:HG2	1:E:57:LEU:HD21	1.99	0.43
1:B:144:ALA:HB1	1:B:151:THR:CG2	2.46	0.43
1:E:230:ASN:HB3	1:E:231:ALA:H	1.55	0.43
1:E:166:GLN:HG2	1:E:195:TYR:CG	2.54	0.43
1:A:38:MET:HE3	2:A:462:HOH:O	2.19	0.43
1:B:163:TYR:HB2	1:B:164:PRO:CD	2.49	0.43
1:C:242:VAL:O	1:C:245:VAL:HG12	2.19	0.43
1:E:220:ILE:HG13	1:E:221:VAL:HG13	2.00	0.43
1:E:166:GLN:HG2	1:E:195:TYR:CD1	2.54	0.43
1:E:199:SER:HB3	1:E:215:MET:CE	2.49	0.43
1:B:247:GLU:O	1:B:250[A]:ARG:HG2	2.19	0.42
1:B:80:GLU:O	1:B:84:LEU:HG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ARG:NH1	2:D:373:HOH:O	2.52	0.42
1:F:145[B]:LYS:HE3	1:F:145[B]:LYS:HB2	1.77	0.42
1:A:56[B]:GLU:OE1	1:A:59:GLY:CA	2.64	0.42
1:C:223:ARG:HH11	1:C:223:ARG:HB3	1.84	0.42
1:D:127[B]:GLU:HG3	1:F:126:MET:SD	2.60	0.42
1:A:105:GLY:HA2	1:A:237[A]:THR:HG22	2.01	0.42
1:F:38:MET:SD	1:F:57[B]:LEU:HG	2.60	0.42
1:E:30[B]:ARG:NH1	1:E:92[B]:ILE:HG13	2.32	0.42
1:A:26:GLY:HA3	2:A:480:HOH:O	2.19	0.42
1:C:205:MET:HB2	1:C:205:MET:HE2	1.83	0.42
1:E:30[B]:ARG:HA	1:E:33:LYS:HD2	2.01	0.42
1:B:57:LEU:HB3	1:B:253:LEU:CD1	2.48	0.41
1:B:199:SER:O	1:B:203:LEU:HG	2.21	0.41
1:D:44:LEU:HD11	1:D:54:ARG:HB2	2.02	0.41
1:E:30[B]:ARG:NH1	1:E:92[B]:ILE:CG1	2.82	0.41
1:A:179:ARG:HG3	2:A:451:HOH:O	2.21	0.41
1:D:253:LEU:HD12	1:D:253:LEU:HA	1.90	0.41
1:F:190:MET:HE1	2:F:444:HOH:O	2.20	0.41
1:F:101:HIS:CE1	2:F:358:HOH:O	2.73	0.41
1:A:87:ARG:HB3	2:A:498:HOH:O	2.21	0.41
1:B:99:GLN:HA	1:B:100:PRO:HD3	1.94	0.41
1:B:96:GLY:HA2	1:B:221:VAL:O	2.21	0.41
1:B:16:LEU:HG	1:B:63:ILE:HG13	2.03	0.41
1:E:57:LEU:HD13	1:E:250[B]:ARG:HG2	2.01	0.41
1:B:138:THR:O	1:B:142[A]:GLU:HG2	2.21	0.41
1:B:48:ARG:HB3	1:B:49[B]:GLU:OE1	2.21	0.41
1:C:24:VAL:HG23	1:C:24:VAL:O	2.21	0.41
1:F:167:GLU:HG2	1:F:169:TYR:CE1	2.56	0.40
1:A:183:SER:HA	1:A:186:GLU:OE1	2.22	0.40
1:F:3:LYS:HD2	2:F:448:HOH:O	2.21	0.40
1:A:215[B]:MET:HG2	1:A:216:VAL:N	2.35	0.40
1:C:33:LYS:HD2	2:C:424:HOH:O	2.21	0.40
1:E:237:THR:HA	2:E:365:HOH:O	2.20	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	268/252 (106%)	264 (98%)	3 (1%)	1 (0%)	39	16
1	B	249/252 (99%)	244 (98%)	4 (2%)	1 (0%)	39	16
1	C	247/252 (98%)	242 (98%)	4 (2%)	1 (0%)	39	16
1	D	251/252 (100%)	247 (98%)	3 (1%)	1 (0%)	39	16
1	E	256/252 (102%)	251 (98%)	3 (1%)	2 (1%)	24	6
1	F	253/252 (100%)	250 (99%)	2 (1%)	1 (0%)	39	16
All	All	1524/1512 (101%)	1498 (98%)	19 (1%)	7 (0%)	34	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	TYR
1	E	231	ALA
1	F	163	TYR
1	A	163	TYR
1	B	163	TYR
1	C	163	TYR
1	E	163	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	219/201 (109%)	216 (99%)	3 (1%)	74	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/201 (101%)	200 (98%)	3 (2%)	72	49
1	C	201/201 (100%)	196 (98%)	5 (2%)	55	25
1	D	205/201 (102%)	200 (98%)	5 (2%)	57	27
1	E	209/201 (104%)	205 (98%)	4 (2%)	65	38
1	F	206/201 (102%)	203 (98%)	3 (2%)	72	49
All	All	1243/1206 (103%)	1220 (98%)	23 (2%)	68	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170[A]	ASP
1	A	170[B]	ASP
1	A	196	GLU
1	B	40	LYS
1	B	196	GLU
1	B	247	GLU
1	C	30[A]	ARG
1	C	30[B]	ARG
1	C	196	GLU
1	C	223	ARG
1	C	225	GLN
1	D	13	LYS
1	D	196	GLU
1	D	238	GLU
1	D	239	SER
1	D	253	LEU
1	E	3	LYS
1	E	92[A]	ILE
1	E	92[B]	ILE
1	E	196	GLU
1	F	3	LYS
1	F	196	GLU
1	F	240	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	D	20	GLN

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Mol	Chain	Res	Type
1	E	225	GLN
1	F	101	HIS
1	F	225	GLN
1	F	240	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 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	252/252 (100%)	-0.21	11 (4%) 38 33	4, 11, 34, 48	12 (4%)
1	B	238/252 (94%)	-0.18	3 (1%) 79 78	6, 17, 33, 48	4 (1%)
1	C	240/252 (95%)	-0.18	9 (3%) 44 40	5, 14, 37, 49	1 (0%)
1	D	244/252 (96%)	-0.33	4 (1%) 74 73	5, 12, 29, 46	1 (0%)
1	E	248/252 (98%)	-0.27	13 (5%) 31 27	4, 11, 34, 46	5 (2%)
1	F	245/252 (97%)	-0.32	5 (2%) 68 67	5, 12, 30, 42	1 (0%)
All	All	1467/1512 (97%)	-0.25	45 (3%) 52 49	4, 13, 33, 49	24 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	THR	11.0
1	E	230	ASN	11.0
1	A	228[A]	ILE	9.6
1	F	231	ALA	8.9
1	B	226	GLN	7.6
1	A	231	ALA	5.2
1	F	239	SER	4.8
1	A	230	ASN	4.5
1	E	234	MET	4.4
1	A	236	GLN	4.3
1	D	230	ASN	4.1
1	C	226	GLN	4.1
1	C	237	THR	4.1
1	A	234	MET	4.0
1	A	2	SER	3.9
1	D	238	GLU	3.8
1	F	2	SER	3.8
1	A	232	GLU	3.7
1	D	253	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	228	ILE	3.6
1	E	226	GLN	3.3
1	E	232	GLU	3.2
1	C	240	HIS	3.2
1	E	233	THR	3.1
1	E	231	ALA	3.1
1	A	235	LYS	3.1
1	B	240	HIS	3.1
1	A	229	PRO	3.1
1	E	236	GLN	3.0
1	C	224	THR	2.8
1	C	238	GLU	2.7
1	F	3	LYS	2.7
1	C	5	ASP	2.6
1	C	101	HIS	2.6
1	F	253	LEU	2.5
1	A	237[A]	THR	2.4
1	C	225	GLN	2.3
1	E	3	LYS	2.3
1	E	235	LYS	2.3
1	E	238	GLU	2.2
1	E	225	GLN	2.2
1	B	7[A]	PHE	2.1
1	C	4	SER	2.1
1	E	240[A]	HIS	2.1
1	E	96	GLY	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.