Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:39 PM GMT

PDB ID	:	4YJK
Title	:	Crystal structure of C212S mutant of Shewanella oneidensis MR-1 uridine phosphorylase
Authors	:	Safonova, T.N.; Mordkovich, N.N.; Manuvera, V.A.; Dorovatovsky, P.V.; Veiko, V.P.; Popov, V.O.; Polyakov, K.M.
Deposited on	:	2015-03-03
Resolution	:	1.68 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

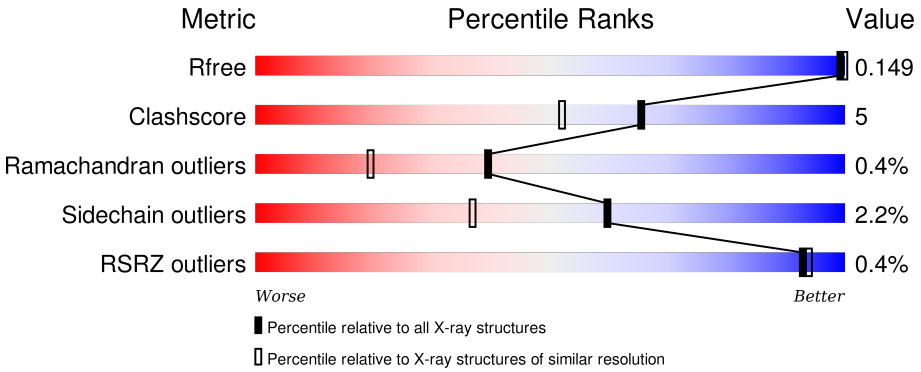
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.68 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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 <=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	% 83% 14% • •
1	B	252	85% 8% • 5%
1	C	252	89% 9% ••
1	D	252	87% 10% ••
1	E	252	% 86% 8% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	252	

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
3	SO4	D	303	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11842 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.

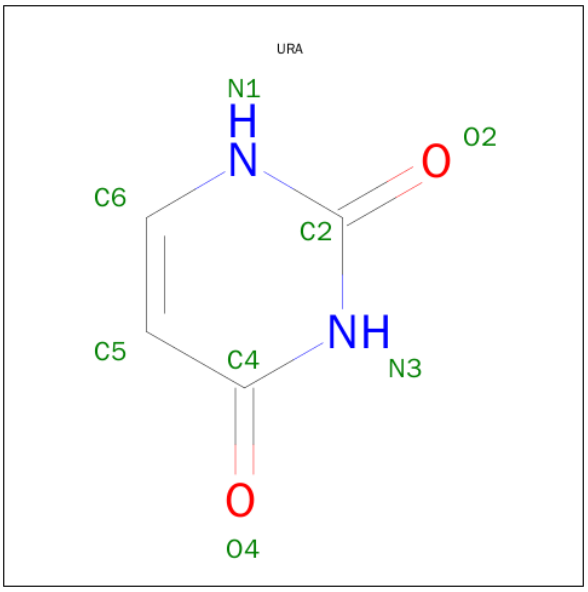
- Molecule 1 is a protein called Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	249	Total	C	N	O	S	0	2	0
			1851	1160	317	361	13			
1	F	244	Total	C	N	O	S	0	1	0
			1817	1141	312	352	12			
1	A	245	Total	C	N	O	S	0	0	0
			1816	1140	313	351	12			
1	C	249	Total	C	N	O	S	0	2	0
			1859	1166	320	360	13			
1	E	242	Total	C	N	O	S	0	1	0
			1796	1128	311	345	12			
1	B	240	Total	C	N	O	S	0	1	0
			1783	1119	310	342	12			

There are 6 discrepancies between the modelled and reference sequences:

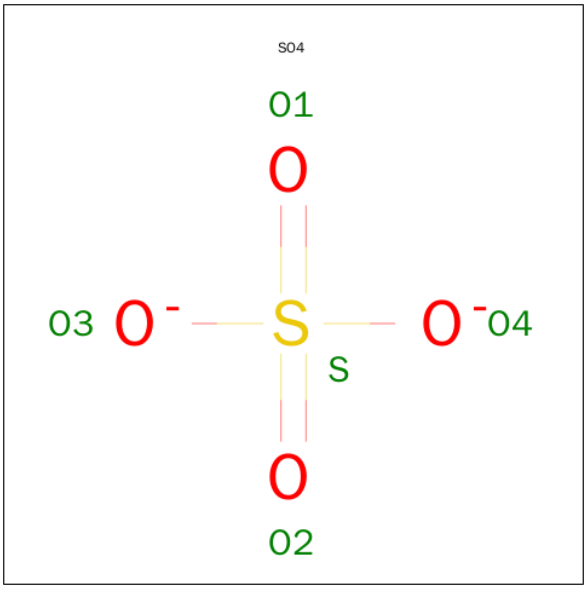
Chain	Residue	Modelled	Actual	Comment	Reference
D	212	SER	CYS	engineered mutation	UNP Q8E9X9
F	212	SER	CYS	engineered mutation	UNP Q8E9X9
A	212	SER	CYS	engineered mutation	UNP Q8E9X9
C	212	SER	CYS	engineered mutation	UNP Q8E9X9
E	212	SER	CYS	engineered mutation	UNP Q8E9X9
B	212	SER	CYS	engineered mutation	UNP Q8E9X9

- Molecule 2 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 10 8 2	0	1
3	F	1	Total O S 5 4 1	0	1
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 10 8 2	0	1
3	E	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

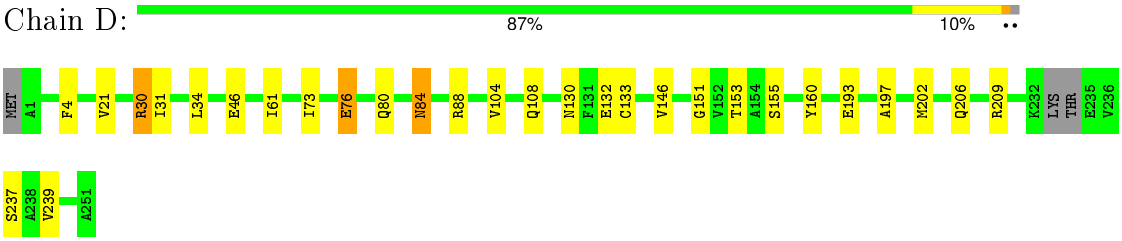
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	149	Total O 149 149	0	0
4	F	138	Total O 138 138	0	0
4	A	151	Total O 151 151	0	0
4	C	149	Total O 149 149	0	0
4	E	129	Total O 129 129	0	0
4	B	125	Total O 125 125	0	0

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.

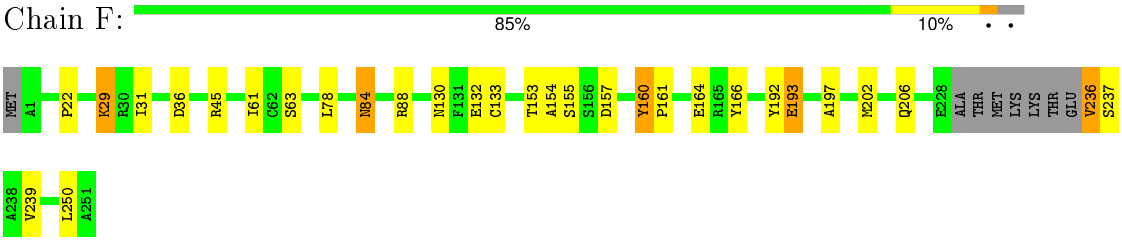
- Molecule 1: Uridine phosphorylase

Chain D:



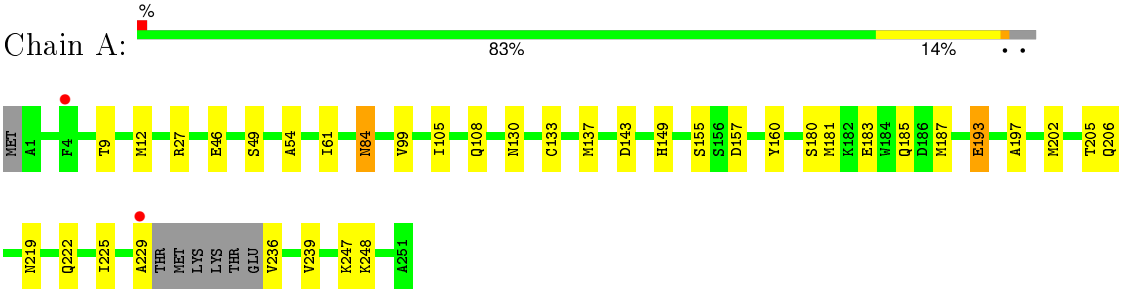
- Molecule 1: Uridine phosphorylase

Chain F:



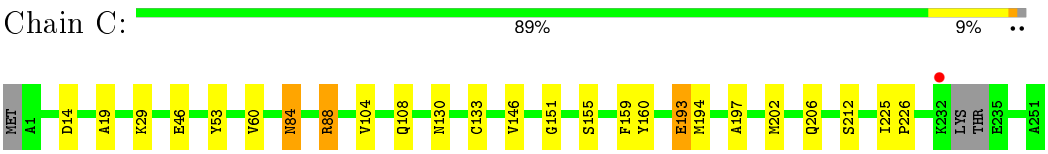
- Molecule 1: Uridine phosphorylase

Chain A:



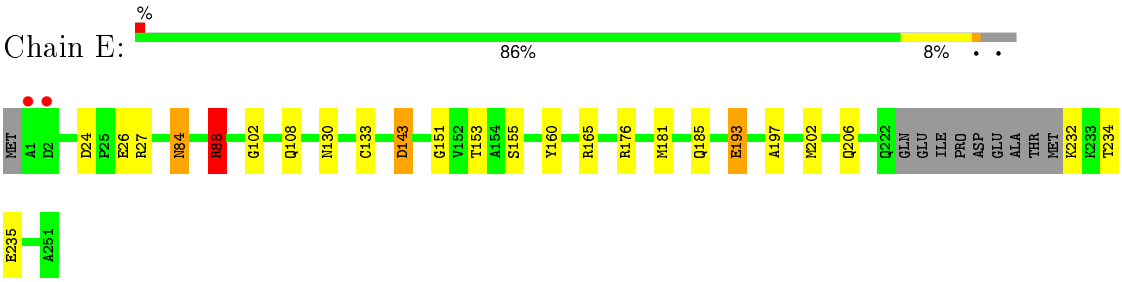
- Molecule 1: Uridine phosphorylase

Chain C:



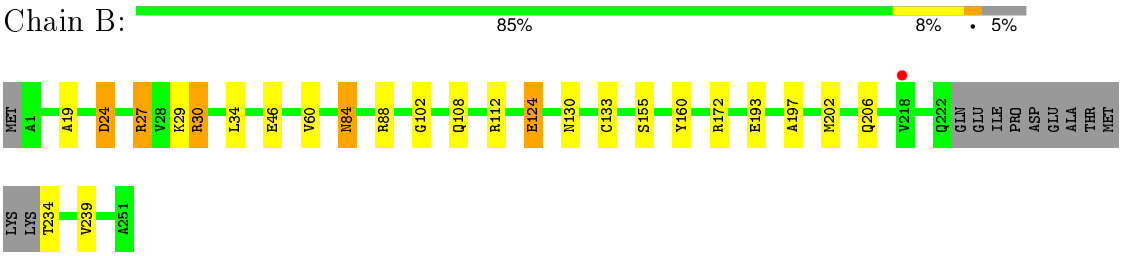
- Molecule 1: Uridine phosphorylase

Chain E:



- Molecule 1: Uridine phosphorylase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.23Å 95.40Å 91.20Å 90.00° 119.98° 90.00°	Depositor
Resolution (Å)	19.35 – 1.68 19.35 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.35-1.68) 98.3 (19.35-1.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.138 , 0.161 0.146 , 0.149	Depositor DCC
R_{free} test set	7594 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	10.8	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.9	EDS
Estimated twinning fraction	0.471 for H, K, L 0.064 for H+L, -K, -L 0.056 for L, -K, H 0.060 for L, K, -H-L 0.182 for -H-L, K, H 0.166 for -H, -K, H+L 0.327 for l,k,-h-l 0.327 for -h-l,k,h 0.257 for -h-l,-k,l 0.286 for h,-k,-h-l 0.246 for l,-k,h	Xtriage
Reported twinning fraction	0.471 for H, K, L 0.064 for H+L, -K, -L 0.056 for L, -K, H 0.060 for L, K, -H-L 0.182 for -H-L, K, H 0.166 for -H, -K, H+L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Outliers	0 of 151174 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11842	wwPDB-VP

Continued on next page...

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

Continued from previous page...

Property	Value	Source
Average B, all atoms ($Å^2$)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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	0.91	0/1848	1.00	2/2514 (0.1%)
1	B	0.91	2/1818 (0.1%)	0.96	2/2471 (0.1%)
1	C	0.92	0/1899	0.99	1/2582 (0.0%)
1	D	0.92	1/1892 (0.1%)	0.99	0/2573
1	E	0.91	0/1831	0.97	3/2490 (0.1%)
1	F	0.92	0/1854	1.01	5/2522 (0.2%)
All	All	0.92	3/11142 (0.0%)	0.99	13/15152 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	GLU	CD-OE2	-7.86	1.17	1.25
1	D	76	GLU	CD-OE2	7.51	1.33	1.25
1	B	124	GLU	CD-OE1	5.17	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	36	ASP	CB-CG-OD1	7.58	125.12	118.30
1	F	157	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	E	88[A]	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	88[B]	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	137	MET	CG-SD-CE	-6.20	90.28	100.20
1	F	78	LEU	CB-CG-CD2	5.95	121.11	111.00
1	B	24	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	157	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	F	36	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	194	MET	CG-SD-CE	5.26	108.62	100.20
1	E	143	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	112	ARG	NE-CZ-NH2	-5.12	117.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	88	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	1816	0	1795	22	0
1	B	1783	0	1769	16	0
1	C	1859	0	1837	21	0
1	D	1851	0	1822	23	0
1	E	1796	0	1779	16	0
1	F	1817	0	1799	16	0
2	A	8	0	3	0	0
2	D	8	0	3	0	0
2	F	8	0	3	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	20	0	0	3	0
3	E	15	0	0	1	0
3	F	5	0	0	0	0
4	A	151	0	0	4	0
4	B	125	0	0	2	0
4	C	149	0	0	5	0
4	D	149	0	0	1	0
4	E	129	0	0	5	0
4	F	138	0	0	1	0
All	All	11842	0	10810	109	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 5.

All (109) 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:D:30:ARG:NH2	3:D:303:SO4:O1	2.05	0.89
1:D:237:SER:HB2	3:D:303:SO4:S	2.21	0.80
1:F:45:ARG:NH2	3:E:302:SO4:O2	2.16	0.79
1:E:27:ARG:NH2	4:E:515:HOH:O	2.18	0.76
1:E:143:ASP:OD1	4:E:401:HOH:O	2.06	0.71
1:A:108:GLN:NE2	4:A:468:HOH:O	2.24	0.70
1:E:130:ASN:HD22	1:E:133:CYS:H	1.38	0.69
1:A:155:SER:HB3	1:A:197:ALA:HB2	1.75	0.69
1:D:130:ASN:HD22	1:D:133:CYS:H	1.41	0.69
1:D:108:GLN:HE21	1:D:151:GLY:HA2	1.59	0.67
1:C:88[A]:ARG:NH2	4:C:532:HOH:O	2.27	0.67
1:A:193:GLU:HB2	4:A:515:HOH:O	1.95	0.65
1:D:202:MET:O	1:D:206:GLN:HG2	1.99	0.63
1:C:193[B]:GLU:OE1	4:C:514:HOH:O	0.63	0.62
1:A:229:ALA:HB3	4:A:525:HOH:O	2.00	0.61
1:A:130:ASN:HD22	1:A:133:CYS:H	1.49	0.61
1:C:130:ASN:HD22	1:C:133:CYS:H	1.48	0.60
1:C:88[A]:ARG:NH2	4:C:531:HOH:O	2.04	0.60
1:B:130:ASN:HD22	1:B:133:CYS:H	1.48	0.60
1:D:155:SER:HB3	1:D:197:ALA:HB2	1.84	0.60
1:A:202:MET:O	1:A:206:GLN:HG2	2.03	0.59
1:E:165:ARG:HD2	4:E:511:HOH:O	2.04	0.58
1:F:130:ASN:HD22	1:F:133:CYS:H	1.52	0.58
1:C:202:MET:O	1:C:206:GLN:HG2	2.03	0.58
1:D:153:THR:HG21	1:D:193[A]:GLU:HG3	1.85	0.57
1:D:84:ASN:C	1:D:84:ASN:HD22	2.08	0.57
1:D:108:GLN:NE2	4:D:504:HOH:O	2.13	0.56
1:D:132:GLU:OE1	1:D:209:ARG:NH1	2.38	0.56
1:A:222:GLN:NE2	4:A:541:HOH:O	2.37	0.56
1:C:84:ASN:C	1:C:84:ASN:HD22	2.08	0.56
1:E:108:GLN:HE21	1:E:151:GLY:HA2	1.71	0.55
1:E:176:ARG:HD2	4:E:439:HOH:O	2.05	0.55
1:D:153:THR:HG21	1:D:193[B]:GLU:HG3	1.88	0.55
1:B:102:GLY:HA2	1:B:234:THR:CG2	2.37	0.55
1:B:84:ASN:C	1:B:84:ASN:HD22	2.10	0.55
1:F:155:SER:HB3	1:F:197:ALA:HB2	1.91	0.53
1:B:27:ARG:NH2	3:B:301:SO4:O4	2.41	0.53
1:C:193[A]:GLU:HB2	4:C:512:HOH:O	2.08	0.53
1:C:19:ALA:HB2	1:C:60:VAL:HG13	1.90	0.53
1:E:84:ASN:C	1:E:84:ASN:HD22	2.12	0.53
1:C:225:ILE:HG22	1:C:226:PRO:O	2.08	0.53
1:C:108:GLN:HE21	1:C:151:GLY:HA2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:SER:HB3	1:E:197:ALA:HB2	1.90	0.53
1:F:202:MET:O	1:F:206:GLN:HG2	2.08	0.52
1:E:232:LYS:HA	1:E:235:GLU:HG3	1.91	0.52
1:B:202:MET:O	1:B:206:GLN:HG2	2.08	0.52
1:D:237:SER:HB2	3:D:303:SO4:O1	2.10	0.52
1:C:88[A]:ARG:HG2	1:C:212:SER:OG	2.10	0.52
1:A:143:ASP:OD2	1:A:248:LYS:NZ	2.28	0.52
1:A:84:ASN:HD22	1:A:84:ASN:C	2.13	0.52
1:C:155:SER:HB3	1:C:197:ALA:HB2	1.92	0.51
1:A:236:VAL:N	1:A:239:VAL:HG22	2.25	0.51
1:D:31:ILE:HG12	1:D:239:VAL:HG13	1.92	0.51
1:B:88[B]:ARG:NH1	4:B:495:HOH:O	0.66	0.51
1:F:61:ILE:HD12	1:F:61:ILE:N	2.26	0.50
1:B:155:SER:HB3	1:B:197:ALA:HB2	1.93	0.50
1:D:104:VAL:HG22	1:D:146:VAL:HG11	1.94	0.50
1:C:19:ALA:HA	1:C:60:VAL:O	2.12	0.49
1:B:30:ARG:CD	4:B:522:HOH:O	2.61	0.49
1:A:9:THR:O	1:A:12:MET:HB2	2.14	0.48
1:A:27:ARG:NH2	3:A:302:SO4:O2	2.42	0.48
1:F:22:PRO:O	1:F:63:SER:HA	2.13	0.48
1:E:130:ASN:ND2	1:E:133:CYS:H	2.11	0.47
1:F:31:ILE:HG12	1:F:239:VAL:HG13	1.97	0.47
1:B:102:GLY:HA2	1:B:234:THR:HG22	1.98	0.46
1:A:181:MET:O	1:A:185:GLN:HG3	2.16	0.46
1:D:4:PHE:CD1	1:C:225:ILE:HG23	2.50	0.45
1:A:183:GLU:O	1:A:187:MET:HG3	2.17	0.45
1:D:46:GLU:HB3	1:C:46:GLU:HB3	1.98	0.45
1:A:54:ALA:HB1	1:A:247:LYS:HG2	1.98	0.45
1:B:24:ASP:CB	1:B:27:ARG:HH21	2.29	0.45
1:F:84:ASN:C	1:F:84:ASN:HD22	2.20	0.45
1:A:99:VAL:O	1:A:219:ASN:ND2	2.50	0.44
1:B:34:LEU:HD12	1:B:239:VAL:HG12	2.00	0.44
1:E:24:ASP:OD1	1:E:26:GLU:HG3	2.18	0.44
1:E:153:THR:HG21	1:E:193:GLU:HG3	2.00	0.43
1:D:73:ILE:HD11	1:C:159:PHE:HB2	1.99	0.43
1:D:34:LEU:CD1	1:D:239:VAL:HG12	2.49	0.43
1:A:49:SER:HA	1:A:61:ILE:O	2.18	0.43
1:C:104:VAL:HG22	1:C:146:VAL:HG11	2.01	0.43
1:D:130:ASN:ND2	1:D:133:CYS:H	2.11	0.42
1:B:19:ALA:HB2	1:B:60:VAL:HG13	2.01	0.42
1:A:130:ASN:ND2	1:A:133:CYS:H	2.15	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88[B]:ARG:NH1	4:E:521:HOH:O	2.36	0.42
1:A:180:SER:O	1:A:183:GLU:HB2	2.20	0.42
1:D:21:VAL:HG23	1:D:88:ARG:HA	2.00	0.42
1:E:202:MET:O	1:E:206:GLN:HG2	2.19	0.42
1:E:102:GLY:HA2	1:E:234:THR:OG1	2.19	0.42
1:D:153:THR:CG2	1:D:193[A]:GLU:HG3	2.50	0.42
1:C:19:ALA:CB	1:C:60:VAL:HG13	2.50	0.41
1:F:164:GLU:HG2	1:F:166:TYR:CE2	2.55	0.41
1:B:102:GLY:HA2	1:B:234:THR:HG21	2.01	0.41
1:F:154:ALA:HB3	1:F:192:TYR:CD1	2.55	0.41
1:A:46:GLU:HB3	1:B:46:GLU:HB3	2.01	0.41
1:F:236:VAL:HA	4:F:524:HOH:O	2.21	0.41
1:B:130:ASN:ND2	1:B:133:CYS:H	2.14	0.41
1:C:130:ASN:ND2	1:C:133:CYS:H	2.17	0.41
1:A:105:ILE:HG12	1:A:149:HIS:HB2	2.01	0.41
1:C:88[A]:ARG:NH1	4:C:531:HOH:O	2.54	0.41
1:F:160:TYR:CB	1:F:161:PRO:CD	2.99	0.41
1:F:160:TYR:HB2	1:F:161:PRO:CD	2.50	0.41
1:C:14:ASP:OD2	1:C:53:TYR:OH	2.30	0.41
1:F:130:ASN:HD21	1:F:132:GLU:HB3	1.86	0.41
1:E:181:MET:O	1:E:185:GLN:HG3	2.21	0.41
1:F:153:THR:HG21	1:F:193[A]:GLU:HG3	2.03	0.41
1:D:76:GLU:O	1:D:80:GLN:HG3	2.20	0.40
1:F:29:LYS:HB3	1:F:29:LYS:HE3	1.88	0.40
1:A:205:THR:O	1:B:172:ARG:NH2	2.55	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	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	39 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	237/252 (94%)	233 (98%)	3 (1%)	1 (0%)	39 19
1	C	247/252 (98%)	240 (97%)	6 (2%)	1 (0%)	39 19
1	D	247/252 (98%)	243 (98%)	3 (1%)	1 (0%)	39 19
1	E	239/252 (95%)	234 (98%)	4 (2%)	1 (0%)	39 19
1	F	241/252 (96%)	234 (97%)	6 (2%)	1 (0%)	39 19
All	All	1452/1512 (96%)	1418 (98%)	28 (2%)	6 (0%)	39 19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	160	TYR
1	A	160	TYR
1	C	160	TYR
1	B	160	TYR
1	F	160	TYR
1	E	160	TYR

5.3.2 Protein sidechains (i)

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	189/198 (96%)	186 (98%)	3 (2%)	70 52
1	B	186/198 (94%)	179 (96%)	7 (4%)	40 15
1	C	195/198 (98%)	189 (97%)	6 (3%)	47 22
1	D	194/198 (98%)	192 (99%)	2 (1%)	82 71
1	E	187/198 (94%)	183 (98%)	4 (2%)	61 39
1	F	191/198 (96%)	184 (96%)	7 (4%)	41 16
All	All	1142/1188 (96%)	1113 (98%)	29 (2%)	60 31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	30	ARG
1	D	84	ASN
1	F	29	LYS
1	F	84	ASN
1	F	193[A]	GLU
1	F	193[B]	GLU
1	F	236	VAL
1	F	237	SER
1	F	250	LEU
1	A	84	ASN
1	A	193	GLU
1	A	225	ILE
1	C	29	LYS
1	C	84	ASN
1	C	88[A]	ARG
1	C	88[B]	ARG
1	C	193[A]	GLU
1	C	193[B]	GLU
1	E	84	ASN
1	E	88[A]	ARG
1	E	88[B]	ARG
1	E	193	GLU
1	B	27	ARG
1	B	29	LYS
1	B	30	ARG
1	B	84	ASN
1	B	108	GLN
1	B	124	GLU
1	B	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	84	ASN
1	D	98	HIS
1	D	108	GLN
1	D	130	ASN
1	D	206	GLN
1	F	84	ASN
1	F	130	ASN
1	F	206	GLN
1	F	222	GLN
1	F	223	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	84	ASN
1	A	98	HIS
1	A	108	GLN
1	A	130	ASN
1	A	222	GLN
1	A	223	GLN
1	C	84	ASN
1	C	108	GLN
1	C	130	ASN
1	E	84	ASN
1	E	108	GLN
1	E	130	ASN
1	B	84	ASN
1	B	130	ASN
1	B	206	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

14 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	URA	A	301	-	4,8,8	1.85	1 (25%)	6,10,10	11.71	4 (66%)
3	SO4	A	302	-	4,4,4	1.26	1 (25%)	6,6,6	0.66	0
3	SO4	B	301	-	4,4,4	0.65	0	6,6,6	0.37	0
3	SO4	C	301	-	4,4,4	0.67	0	6,6,6	0.40	0
2	URA	D	301	-	4,8,8	1.94	2 (50%)	6,10,10	11.68	4 (66%)
3	SO4	D	302	-	4,4,4	1.04	1 (25%)	6,6,6	0.47	0
3	SO4	D	303	-	4,4,4	0.40	0	6,6,6	0.90	1 (16%)
3	SO4	D	304[A]	-	4,4,4	0.38	0	6,6,6	0.26	0
3	SO4	D	304[B]	-	4,4,4	0.23	0	6,6,6	0.73	0
3	SO4	E	301[A]	-	4,4,4	0.34	0	6,6,6	0.24	0
3	SO4	E	301[B]	-	4,4,4	0.38	0	6,6,6	0.38	0
3	SO4	E	302	-	4,4,4	0.35	0	6,6,6	0.79	0
2	URA	F	301	-	4,8,8	1.74	1 (25%)	6,10,10	11.49	4 (66%)
3	SO4	F	302[A]	-	4,4,4	1.31	0	6,6,6	0.70	0

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	URA	A	301	-	-	0/0/0/0	0/1/1/1
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
3	SO4	B	301	-	-	0/0/0/0	0/0/0/0
3	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	URA	D	301	-	-	0/0/0/0	0/1/1/1
3	SO4	D	302	-	-	0/0/0/0	0/0/0/0
3	SO4	D	303	-	-	0/0/0/0	0/0/0/0
3	SO4	D	304[A]	-	-	0/0/0/0	0/0/0/0
3	SO4	D	304[B]	-	-	0/0/0/0	0/0/0/0
3	SO4	E	301[A]	-	-	0/0/0/0	0/0/0/0
3	SO4	E	301[B]	-	-	0/0/0/0	0/0/0/0
3	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	URA	F	301	-	-	0/0/0/0	0/1/1/1
3	SO4	F	302[A]	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	URA	C5-C6	-2.07	1.34	1.38
3	A	302	SO4	O3-S	2.04	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	SO4	O2-S	2.08	1.54	1.47
2	F	301	URA	C4-N3	2.58	1.37	1.33
2	D	301	URA	C4-N3	2.72	1.38	1.33
2	A	301	URA	C4-N3	2.76	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	URA	N1-C2-N3	-21.22	114.79	128.33
2	A	301	URA	N1-C2-N3	-21.20	114.81	128.33
2	F	301	URA	N1-C2-N3	-20.80	115.06	128.33
2	D	301	URA	C5-C4-N3	-3.37	114.46	123.12
2	A	301	URA	C5-C4-N3	-3.36	114.50	123.12
2	F	301	URA	C5-C4-N3	-3.36	114.51	123.12
3	D	303	SO4	O4-S-O3	2.07	117.40	108.98
2	F	301	URA	C6-N1-C2	13.09	120.84	114.40
2	F	301	URA	C4-N3-C2	13.19	127.20	114.14
2	D	301	URA	C6-N1-C2	13.21	120.90	114.40
2	A	301	URA	C4-N3-C2	13.24	127.25	114.14
2	D	301	URA	C4-N3-C2	13.39	127.40	114.14
2	A	301	URA	C6-N1-C2	13.53	121.06	114.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SO4	1	0
3	B	301	SO4	1	0
3	D	303	SO4	3	0
3	E	302	SO4	1	0

5.7 Other polymers (i)

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^{th} 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	245/252 (97%)	-0.36	2 (0%) 87 89	8, 13, 24, 39	0
1	B	240/252 (95%)	-0.30	1 (0%) 93 94	8, 14, 28, 37	0
1	C	249/252 (98%)	-0.37	1 (0%) 93 94	7, 13, 23, 41	0
1	D	249/252 (98%)	-0.39	0 100 100	8, 13, 23, 42	0
1	E	242/252 (96%)	-0.34	2 (0%) 87 89	8, 13, 24, 41	0
1	F	244/252 (96%)	-0.38	0 100 100	8, 13, 24, 31	0
All	All	1469/1512 (97%)	-0.36	6 (0%) 93 94	7, 13, 25, 42	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	4.5
1	E	2	ASP	2.9
1	B	218	VAL	2.7
1	A	229	ALA	2.6
1	A	4	PHE	2.5
1	C	232	LYS	2.3

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

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^{th} 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
3	SO4	E	302	5/5	0.91	0.17	1.10	21,21,23,23	5
3	SO4	C	301	5/5	0.91	0.12	0.89	13,14,14,15	5
3	SO4	B	301	5/5	0.92	0.12	0.81	18,20,21,21	5
3	SO4	A	302	5/5	0.98	0.09	0.75	16,17,19,20	0
2	URA	D	301	8/8	0.97	0.07	-0.44	13,14,14,15	0
2	URA	A	301	8/8	0.96	0.07	-0.70	14,16,17,19	0
2	URA	F	301	8/8	0.96	0.07	-1.20	12,13,13,15	0
3	SO4	F	302[A]	5/5	0.98	0.06	-1.75	13,14,14,16	1
3	SO4	D	302	5/5	0.99	0.04	-2.15	17,17,18,19	0
3	SO4	D	304[B]	5/5	0.99	0.06	-	14,14,15,15	5
3	SO4	E	301[B]	5/5	0.98	0.08	-	16,16,17,18	5
3	SO4	E	301[A]	5/5	0.98	0.08	-	17,18,19,20	5
3	SO4	D	304[A]	5/5	0.99	0.06	-	17,18,18,18	5
3	SO4	D	303	5/5	0.95	0.13	-	23,23,24,25	5

6.5 Other polymers

There are no such residues in this entry.